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On the Space-Time Formulation of Non-Relativistic Quantum Mechanics

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For the case of the quantization of the usual non-relativistic classical Lagrangian function quadratic in the velocity the validity is demonstrated of the non-canonical space-time formulation of quantum mechanics proposed recently by the author, which aims to evaluate, without appealing to the Schrödinger equation, the transformation function $K(x, t''; y, t')$ in the space representation on the basis of the composition rule

$$K(x, t''; y, t') = \int K(x, t''; z, t)\, dz\, K(z, t; y, t') \tag{1}$$

coupled with the supposition that it is approximated to zeroth order in the quantum of action h by the so-called semi-classical kernel

$$K_c(x, t''; y, t') = [(i/h)\partial^2 S/\partial x \partial y]^{1/2} \exp[(i/\hbar) S(x, t''; y, t')] \tag{2}$$

written in terms of the classical action $S(x, t''; y, t')$ alone.

In the first place the action function corresponding to the above Lagrangian is expanded in power of the interval of time $T = t'' - t'$. Then the deviation of the semi-classical kernel (2) from the unitary transformation function is shown to be of the third order in T, and the corresponding correction term is evaluated by solving the integral equation (1). It is also shown that the semi-classical kernel is unitary for a free motion of a particle with its mass being a function in the space coordinate.

§ 1. Introduction and summary

In quantum mechanics the temporal development of a physical system is described essentially by the transformation function or the kernel $K(x, t; y, t')$, such that for $t = t'$

$$K(x, t; y, t) = \delta(x - y). \tag{1·1}$$

In the traditional formulation this is a solution of the Schrödinger equation

$$i\hbar(\partial/\partial t) K(x, t; y, t') = H(x, p, t) K(x, t; y, t'), \tag{1·2}$$

where p denotes the differential operator $-i\hbar(\partial/\partial x)$. If $\partial H/\partial t = 0$, the solution reads simply with $T = t - t'$

$$K(x, y, T) = \exp[-(iT/\hbar) H(x, p)]\delta(x - y). \tag{1·3}$$

In this canonical formalism the Hamiltonian operator plays an essential part, which is constructed on the basis of a kind of formal correspondence with the Hamiltonian function $H(q, p, t)$ in classical mechanics, where q and p denote the space coordinate of a particle and its canonically conjugate momentum, respectively.

In contrast with this, Feynman's space-time version of quantum mechanics[1] aimed to establish, without the use of canonical variables, an equivalent and self-contained theoretical scheme in the usual space-time framework. The superiority of this approach starting from the classical action function to the usual one consists in securing a direct correspondence of quantum mechanical description with the classical mechanical one formulated originally in the form of Hamilton's principle of stationary action in the usual space-time.

Feynman's formulation suffered, however, from the drawback, as was pointed out by himself, that it required an unnatural and cumbersome infinite subdivision of the time interval T. This is not only true from the side of mathematical conceptions needed therein, but also from the practical point of view of the actual integration of the transformation function. The exact realization of Feynman's recipe has so far been limited to the simple and trivial cases of the free particle and the harmonic oscillator alone and no practical method of integration has been devised applicable to wider class of action functionals.[2]

In the present paper the following two things are shown in the non-relativistic quantum mechanics of a particle of mass m moving in one space dimension, whose classical Lagrangian and Hamiltonian functions are given respectively by

$$L(q,\, v) = (m/2)\, v^2 - V(q) \tag{1·4}$$

and by

$$H(q,\, p) = (1/2m)\, p^2 + V(q), \tag{1·5}$$

where v denotes the velocity $dq(t)/dt$. In the first place it is possible to construct a space-time formulation of quantum mechanics without appealing to an infinite subdivision of the interval of time. In the second place it becomes thus possible to evaluate the transformation function, when the potential $V(q)$ is given arbitrarily. In order to make clear the differences between the fundamental postulates underlying the present formulation and those in Feynman's, it is needed first to analyse the essentials of the so-called Feynman principle.

Let $q(t)$ represent a classical path of a particle connecting a pair of space-time points (x, t'') and (y, t'), then $x=q(t'')$ and $y=q(t')$. This function $q(t)$ is determined by the variation principle

$$\delta \int_{t'}^{t''} dt\, L[q(t)\,,\, v(t),\, t] = 0, \tag{1·6}$$

or equivalently by the Lagrangian equation of motion

$$(d/dt)\,\partial L/\partial v = \partial L/\partial q, \tag{1·7}$$

and the time integral of the Lagrangian function

$$S(x,\, t''\,;\, y,\, t') = \int_{t'}^{t''} dt\, L[q(t),\, v(t),\, t] \tag{1·8}$$

along the actual classical path is called the classical action function. From the very beginning of quantum mechanics the relation of this function to quantum mechanics has repeatedly been emphasized by various authors.[3] Especially Van Vleck showed that the transformation function could be approximated to zeroth order in the quantum of action h by the semi-classical kernel

$$K_c(x, t; y, t') = [(i/h)\partial^2 S/\partial x\partial y]^{1/2} \exp[(i/\hbar)S(x, t; y, t')] \tag{1·9}$$

constructed from the classical action alone.[4] Of course this can not in general represent a unitary transformation. But in some favourable cases it happens that this is correct to the first order in the time interval $T=t-t'$, or more precisely that, supposing $\partial H/\partial t=0$,

$$K_c(x, y, T) = [1-(iT/\hbar)H(x, p)]\delta(x-y) + O(T^2). \tag{1·10}$$

Now it is well known that any finite unitary transformation is a result of an infinite unfolding of successive infinitesimal unitary transformations. It was thus asserted by Feynman that, when and only when the semi-classical kernel is correct to the first order in T, the infinite unfolding of infinitesimal unitary transformations goes over to the functional integration method

$$K(x, t; y, t') = \int d(\text{paths}) \exp[(i/\hbar)S(\text{path})] \tag{1·11}$$

over all possible imaginary paths in space-time with the common end points (x, t) and (y, t'), of which the result will be the same with that of the Schrödinger equation. The reason for this was stated as follows. If a given finite interval of time, T^*, is subdivided into equal steps T, the number of the factors of the form (1·10) is T^*/T. If an error of order T^2 is made in each, the resulting error will not accumulate beyond the order $T^2(T^*/T)$ or T^*T, which vanishes in the limit $T\to 0$.

This is actually the case for the non-relativistic quantum mechanics corresponding to the classical system characterized by (1·4) and (1·5). Feynman showed this by establishing, with the aid of the approximation formula

$$S(x, y, T) = (m/2T)(x-y)^2 - TV(x) \tag{1·12}$$

to the classical action function (1·8), the relationship

$$\int dy\, K_c(x, y, T)\psi(y) = [1-(iT/\hbar)H(x, p)]\psi(x) + O(T^2), \tag{1·13}$$

which is equivalent to the above (1·10). In this connection the question arises to what extent the semi-classical kernel is a correct one in the non-relativistic case now under consideration. The following three sections will thus be devoted to the improvement of the approximation formula (1·12) yielding the result

$$S(x, y, T) = (m/2T)(x-y)^2 - TF_1(x, y) - (T^3/2m)F_3(x, y) + O(T^5), \tag{1·14}$$

wherein

$$F_1(x, y) = \int_0^1 du\, V[y+u(x-y)] \tag{1·15}$$

and the expression for $F_3(x, y)$ will be found in (3·22). It will then be shown in § 5 that (1·10) will accordingly be changed to the form

$$K_c(x, y, T) = K(x, y, T) - (i\hbar T^3/240m^2)[(d/dx)^4 V(x)]\delta(x-y) + O(T^4) \tag{1·16}$$

with the $K(x, y, T)$ given by (1·3). The semi-classical kernel is, therefore, correct to the second order in T and the transformation function should be written in the form

$$\begin{aligned} K(x, y, T) &= K_c(x, y, T)[1 + (i\hbar T^3/8m^2) D(x, y) + O(T^4)] \\ &= K_c(x, y, T) + (i\hbar T^3/8m^2) D(x, x)\delta(x-y) + O(T^4). \end{aligned} \tag{1·17}$$

Comparing this with the above (1·16), we get at once the condition

$$D(x, x) = (1/30)\,(d/dx)^4 V(x). \tag{1·18}$$

The task of the space-time formulation of quantum mechanics will thus be to determine the unknown function $D(x, y)$ subjected to the condition (1·18) without relying upon the Schrödinger equation.

It is evident from the above that the Feynman principle is correct at least in principle so far as we are concerned with the non-relativistic Lagrangian (1·4). But being hindered by mathematical difficulties, no attempt has so far been made to obtain by this method the function $D(x, y)$ in the general case of an arbitrary potential $V(q)$. Apart from this difficulty the limitation is inherent in Feynman's method that it is valid only for the restricted class of action functionals, for which the corresponding semi-classical kernels are correct to the first order in the time interval. Therefore, as far as the correspondence with the classical mechanical picture is made via the semi-classical kernel written in terms of the classical action functional, the most general form of the space-time formulation of quantum mechanics applicable also to wider class of action functionals will essentially be at variance with an infinite subdivision of the interval of time.

Now in so far as the parameter h is concerned alone, the semi-classical kernel is correct to the zeroth order in it for any finite interval of time. The unitarity of the transformation function will thus be secured by putting

$$K(x, t; y, t') = K_c(x, t; y, t')\, U(x, t; y, t') \tag{1·19}$$

with the correction factor $U(x, t; y, t')$ such that

$$\lim_{\hbar\to 0} U(x, t; y, t') = 1. \tag{1·20}$$

Then in our non-relativistic case we have from (1·17)

$$U(x, y, T) = 1 + i\hbar[(T^3/8m^2) D(x, y) + O(T^4)] + O(\hbar^2). \tag{1·21}$$

But for the purpose of determining the unknown factor $U(x, t; y, t')$ the use of the unitarity condition

$$\int dz\, K(x, t; z, t')K(y, t; z, t')^* = \delta(x-y), \tag{1·22}$$

where the asterisk denotes the complex conjugate, is inconvenient, because the delta-function in the right-hand side is mathematically hard to manipulate. Therefore, the author has recently proposed[5] to base the space-time formulation of quantum mechanics on the use of the recursive condition

$$K(x, t''; y, t') = \int K(x, t''; z, t)\, dz\, K(z, t; y, t'), \tag{1·23}$$

which yields the above (1·22) for $t''=t'$ according to (1·1). The final object of the present paper is thus to show that this recipe for the construction of the transformation function works well at least in the non-relativistic case wherein the action function is approximately given by (1·14). In § 6 the integral equation (1·23) is solved to determine the function $D(x, y)$ in (1·21) as

$$D(x, y) = (\partial^2/\partial x\partial y)^2 F_1(x, y) \tag{1·24}$$

in terms of $F_1(x, y)$ given in (1·15). This at once gives

$$D(x, x) = \int_0^1 du\, u^2(1-u)^2(d/dx)^4 V(x), \tag{1·25}$$

which is nothing but the condition (1·18). In addition to this it will be shown in § 7 that the semi-classical kernel corresponding to the classical Lagrangian function

$$L(q, v) = (m/2)[w(q)v]^2 \tag{1·26}$$

will itself satisfy the recursive condition (1·23). Therefore the semi-classical kernel is unitary and we can put in this case the function U in (1·19) equal to unity.

Now from the above one may safely expect that the space-time formulation of quantum mechanics based on the coupled use of the recursive condition (1·23) and the factorization (1·19) of the transformation function in terms of the semi-classical kernel (1·9) is valid in general for wider class of action functionals. In order to show that this is actually the case, it is needed first to devise some mathematical transformation of the condition (1·23) into a more tractable one and then to utilize it in quantizing classical systems different essentially from those treated in this paper. Moreover, in order that the present formulation should be a complete and self-contained one, or more precisely that it should be completely free from the influence of the Schrödinger equation, one has to be able to explain, in the framework of the recursive condition alone, the reason why one is to start from the factorization (1·19). This means, as has already been pointed out by the author,[5] that the principle of correspondence with the classical mechanical description is to be implied, in the limit of the quantum of action h tending to zero, in the recursive condition representing the group property of the transformation function. In addition to these it will be of interest to investigate what condition is imposed on the classical Lagrangian function in order that the semi-classical kernel is correct to the first order in the time interval or accordingly that the passage to Feynman's path integral method of quantization is really possible. These are the problems left to be solved and the solutions will be given in succeeding papers.

§ 2. Evaluation of action function by the Hamilton-Jacobi equation

Since the Lagrangian function (1·4) does not depend explicitly on the time t, the action function (1·8) involves t'' and t' in the form of the difference $T=t''-t'$ and can accordingly be written as $S(x, y, T)$. In the case of free motion with vanishing potential it reads simply

$$S_f(x, y, T)=(m/2T)(x-y)^2. \tag{2·1}$$

When the particle is acted on by force, the explicit construction of action function is difficult to perform and it has so far been successful only for the restricted cases, where the potential is linear or quadratic in the coordinate. For

$$V(q)=kq \qquad \text{and} \qquad V(q)=(m\omega^2/2)q^2 \tag{2·2}$$

with the constants k and ω, the results are respectively

$$S(x, y, T)=S_f(x, y, T)-(k/2)T(x+y)-(k^2/24m)T^3 \tag{2·3}$$

and

$$\begin{aligned} S(x, y, T)&=(m\omega/2\sin\omega T)[(x^2+y^2)\cos\omega T-2xy] \\ &=S_f(x, y, T)-(m\omega^2/6)T(x^2+xy+y^2) \\ &\quad-(m\omega^4/90)T^3[x^2+(7/4)xy+y^2]-\cdots. \end{aligned} \tag{2·4}$$

It is common to these that the first term $S_f(x, y, T)$ is followed by the terms of odd power in T, so that we put in the general case of an arbitrary potential $V(q)$

$$S(x, y, T)=S_f(x, y, T)-TF(x, y, T) \tag{2·5}$$

with

$$F(x, y, T)=\sum_{k=0}^{\infty}(T^2/2m)^k F_{2k+1}(x, y). \tag{2·6}$$

The Hamilton-Jacobi equation derived from the Hamiltonian function (1·5) is

$$(\partial/\partial T)S(x, y, T)+(1/2m)[(\partial/\partial x)S(x, y, T)]^2+V(x)=0, \tag{2·7}$$

which is transcribed with $a=T^2/2m$ as

$$\sum_{n=0}^{\infty}a^n(x-y)^{-2n}(\partial/\partial x)[(x-y)^{2n+1}F_{2n+1}(x, y)]=\sum_{n=0}^{\infty}a^n G_{2n}(x, y), \tag{2·8}$$

where

$$G_0(x, y)=V(x) \tag{2·9}$$

and

$$G_{2n}(x, y)=\sum_{k=0}^{n-1}(\partial/\partial x)F_{2k+1}\cdot(\partial/\partial x)F_{2n-(2k+1)}, \quad (n>0). \tag{2·10}$$

The solutions are given at once by

$$F_{2n+1}(x,\ y)=(x-y)^{-(2n+1)}[\int_y^x dz(z-y)^{2n}G_{2n}(z,\ y)+C_{2n+1}(y)]$$
$$=\int_0^1 du\ u^{2n}G_{2n}[g(u),\ y]+(x-y)^{-(2n+1)}C_{2n+1}(y), \qquad (2\cdot 11)$$

where we have replaced z with $g(u)=y+u(x-y)$ and $C_{2n+1}(y)$ are the integration constants.

According to the definition (1·8) of the classical action, the term of the lowest order in T should be $TL(q,\ v)$, when the substitutions $y=q$ and $x-y=vT$ are made in it. But from the above we get

$$S(q+vT,\ q,\ T)=-\sum_{k=0}^{\infty}(2m)^{-k}v^{-(2k+1)}C_{2k+1}(q)+O(T), \qquad (2\cdot 12)$$

so we must put $C_{2n+1}(y)=0$ in (2·11). Then for $n=0$ we get the solution (1·15) according to (2·9) and for $n=1$ we have from (2·10) and (2·11) respectively with the abbreviations $V_k(x)=(d/dx)^k V(x)$

$$G_2(x,\ y)=[(\partial/\partial x)F_1(x,\ y)]^2=[\int_0^1 dw\ w\ V_1[g(w)]]^2, \qquad (2\cdot 13)$$

$$F_3(x,\ y)=\int_0^1 du\ u^2 G_2[g(u),\ y]=\int_0^1 du\ u^2[\int_0^1 dw\ w\ V_1[g(uw)]]^2$$
$$=\int_0^1 du\ \{(1/u)\int_0^u dw\ w\ V_1[g(w)]\}^2. \qquad (2\cdot 14)$$

The results in this section were obtained by the author[6] in 1950 and essentially the same results were also attained afterwards in 1955 by Choquard.[7] Instead of adopting a roundabout method based on the partial differential equation (2·7) we had, however, better to construct the classical action directly according to its original definition (1·8). The next section will thus be devoted to this purpose.

§ 3. Evaluation of action function by direct integration

The classical path $q(t)$ of a particle, whose Lagrangian function is given by (1·4), is determined by the Newtonian equation of motion

$$m(d/dt)^2 q(t)=-V_1[q(t)] \qquad (3\cdot 1)$$

derived from (1·7) and in addition to this by the initial conditions $x=q(t'')$ and $y=q(t')$. Then in terms of a real parameter u defined by $t=t'+u(t''-t')$ the classical path is represented by a function $q(u)$, such that $x=q(1)$ and $y=q(0)$, and at the same time the above equation is rewritten as

$$q''(u)=-2aV_1[q(u)], \qquad (3\cdot 2)$$

where $a=T^2/2m$ and the prime denotes the differentiation with respect to the parameter u.

In the case of a free motion the solution $q(u)$ is at once given by $g(u)=y+u\xi$ with $g'(u)=\xi=x-y$ and $g''(u)=0$. Then putting in the general case of an arbitrary potential $V(q)$

$$q(u)=g(u)+f(u), \tag{3·3}$$

we get $f(1)=f(0)=0$ and from (3·2) the equation

$$\begin{aligned}(-1/2a)f''(u)&=V_1[g(u)+f(u)]\\&=V_1[g(u)]+V_2[g(u)]f(u)+(1/2)V_3[g(u)]f(u)^2+\cdots.\end{aligned} \tag{3·4}$$

The expansion of $f(u)$ in powers of a

$$f(u)=\sum_{k=1}^{\infty}(-2a)^k f_{2k}(u) \tag{3·5}$$

gives $f_{2k}(1)=f_{2k}(0)=0$ and transforms the above (3·4) into

$$f_2''(u)=V_1[g(u)]=(1/\xi)(d/du)V[g(u)], \tag{3·6}$$

$$f_4''(u)=V_2[g(u)]f_2(u), \tag{3·7}$$

$$f_6''(u)=V_2[g(u)]f_4(u)+(1/2)V_3[g(u)]f_2(u)^2, \tag{3·8}$$

and so on. After repeated differentiations (3·6) gives

$$f_2^{(n+1)}(u)=\xi^{n-1}V_n[g(u)] \tag{3·9}$$

and accordingly (3·7) and (3·8) are transformed respectively into

$$\begin{aligned}\xi f_4''(u)&=\xi V_2[g(u)]f_2(u)=f_2^{(3)}(u)f_2(u)\\&=[f_2'(u)f_2(u)]''-(3/2)[f_2'(u)^2]',\end{aligned} \tag{3·10}$$

$$\begin{aligned}2\xi f_6''(u)&=2f_2^{(3)}(u)f_4(u)+(1/\xi)f_2^{(4)}(u)f_2(u)^2\\&=[f_2(u)f_4'(u)-3f_2'(u)f_4(u)]''+5[f_2''(u)f_4(u)]'.\end{aligned} \tag{3·11}$$

Now (3·6) is at once integrated to give

$$f_2(u)=(1/\xi)\Big[\int_0^u-u\int_0^1\Big]dw\,V[g(w)] \tag{3·12}$$

$$=(1/\xi)u\int_0^1 dw\,\{V[g(uw)]-V[g(w)]\} \tag{3·13}$$

and in the same way we get from (3·10) and (3·11)

$$\xi f_4(u)=f_2'(u)f_2(u)-(3/2)\Big[\int_0^u-u\int_0^1\Big]dw\,f_2'(w)^2, \tag{3·14}$$

$$2\xi f_6(u)=f_2(u)f_4'(u)-3f_2'(u)f_4(u)+5\Big[\int_0^u-u\int_0^1\Big]dw f_2''(w)f_4(w). \tag{3·15}$$

According to the above results the Lagrangian function (1·4) is transcribed as

$$\begin{aligned}L(q,v)&=(m/2T^2)[g'(u)+f'(u)]^2-V[q(u)]\\&=(1/T)S_f(x,y,T)-D(u)+(d/du)C(u)\end{aligned} \tag{3·16}$$

with
$$D(u)=V[q(u)]+(m/2T^2)f(u)f''(u)$$
$$=V[g(u)+f(u)]-(1/2)f(u)V_1[g(u)+f(u)] \tag{3·17}$$
and
$$C(u)=(m/2T^2)f(u)[2(x-y)+f'(u)], \tag{3·18}$$
which gives $C(1)=C(0)=0$. Then we get from (3·17)

$$D(u)-V[g(u)]=(1/2)\sum_{n=1}^{\infty}(1/n!)(2-n)V_n[g(u)]f(u)^n$$
$$=(1/2)\sum_{n=1}^{\infty}(1/n!\,\xi^{n-1})(2-n)f_2^{(n+1)}(u)f(u)^n$$
$$=(1/2)f_2''(u)f(u)-(1/12\xi^2)f_2^{(4)}(u)f(u)^3+\cdots$$
$$=-af_2''(u)f_2(u)+2a^2f_2''(u)f_4(u)+O(a^3) \tag{3·19}$$

and accordingly
$$D(u)=V[g(u)]+a[f_2'(u)^2-(f_2f_2')'] \tag{3·20}$$
$$+a^2(2/\xi)[f_2'(u)^3+(f_2^2f_2''-f_2f_2'^2)'+\xi(f_2'f_4-f_2f_4')']+O(a^3).$$

Since (1·8) gives, with the aid of (3·16) and (3·18),
$$S(x,y,T)=T\int_0^1 du\,L[q(u),v(u)]=S_f(x,y,T)-T\int_0^1 du\,D(u), \tag{3·21}$$
one has, according to (2·5), (2·6), (3·20) and (3·12), in the first place the result (1·15) and then
$$F_3(x,y)=\int_0^1 du\,f_2'(u)^2$$
$$=(1/\xi)^2\Big[\int_0^1 du\,V[g(u)]^2-\Big\{\int_0^1 du\,V[g(u)]\Big\}^2\Big], \tag{3·22}$$
$$F_5(x,y)=(2/\xi)\int_0^1 du\,f_2'(u)^3. \tag{3·23}$$

Finally according to (3·6) one has
$$\Big[(1/u)\int_0^u dw\,w\,V_1[g(w)]\Big]^2=\Big[(1/u)\int_0^u dw\,w\,f_2''(w)\Big]^2$$
$$=[f_2'(u)-(1/u)f_2(u)]^2=f_2'(u)^2-(d/du)[(1/u)f_2(u)^2], \tag{3·24}$$
and since $(1/u)f_2(u)^2$ vanishes both for $u=0$ and for $u=1$ owing to (3·13), we see that (3·22) is identical with (2·14).

§ 4. Some properties of action function

Let a function $q(t)$ with $q(t'')=x$ and $q(t')=y$ represent a classical path $P(x,t'';y,t')$ of a particle and let an imaginary path, which is composed of two classical paths $P(x,t'';q^*,t^*)$ and $P(q^*,t^*;y,t')$ jointed together at (q^*,t^*), be represented by a varied function $q(t)+\delta q(t)$, then we have $\delta q(t'')=\delta q(t')=0$ and $\delta q(t^*)=q^*-q(t^*)$. The definition (1·8) of the classical action gives now

$$S(x, t''; q^*, t^*)+S(q^*, t^*; y, t')-S(x, t''; y, t')$$
$$=\int_{t'}^{t''}dt\, L(q+\delta q, v+\delta v, t)-\int_{t'}^{t''}dt\, L(q, v, t) \tag{4·1}$$

and taking up to the first order variation the right-hand side vanishes owing to (1·6), so that from the expansion of the left-hand side in $\delta q(t^*)$, we get, by putting $z=q(t)$, the following two conditions,

$$S(x, t''; y, t')=S(x, t''; z, t)+S(z, t; y, t') \tag{4·2}$$

and

$$(\partial/\partial z)[S(x, t''; z, t)+S(z, t; y, t')]=0. \tag{4·3}$$

In the case of a free motion the classical path $q(t)$ is given by $g(u)=ux+wy$ with $w=1-u$, and for the classical action (2·1) we have the relationship

$$S_f(x, z, wT)+S_f(z, y, uT)-S_f(x, y, T)$$
$$=(m/2uwT)[z-g(u)]^2=S_f[z, g(u), uwT], \tag{4·4}$$

where z is taken arbitrarily. Then for $z=g(u)$ the above conditions (4·2) and (4·3) are easily seen to be fulfilled. In the general case of an arbitrary potential $V(q)$ they are rewritten with the aid of (2·5) and (4·4) respectively as

$$wF(x, z, wT)+uF(z, y, uT)-F(x, y, T)=(1/4uwa)[z-g(u)]^2 \tag{4·5}$$

and

$$(\partial/\partial z)[wF(x, z, wT)+uF(z, y, uT)]=(1/2uwa)[z-g(u)], \tag{4·6}$$

where z is given according to (3·3) and (3·5) by $z=g(u)-2af_2(u)+O(a^2)$. Then in view of the expansion $F(x, y, T)=F_1(x, y)+aF_3(x, y)+O(a^2)$ given in (2·6) the condition (4·5) gives with the abbreviation $\langle\varphi(x, y, z)\rangle=\varphi[x, y, g(u)]$

$$\langle wF_1(x, z)+uF_1(z, y)\rangle-F_1(x, y)=0 \tag{4·7}$$

and

$$\langle w^3F_3(x, z)+u^3F_3(z, y)\rangle-F_3(x, y)$$
$$=2f_2(u)\langle(\partial/\partial z)[wF_1(x, z)+uF_1(z, y)]\rangle+(1/uw)f_2(u)^2. \tag{4·8}$$

In the same way the condition (4·6) yields

$$\langle(\partial/\partial z)[wF_1(x, z)+uF_1(z, y)]\rangle=-(1/uw)f_2(u), \tag{4·9}$$

which transforms (4·8) into

$$F_3(x, y)-\langle w^3F_3(x, z)+u^3F_3(z, y)\rangle=uw\langle(\partial/\partial z)[wF_1(x, z)+uF_1(z, y)]\rangle^2. \tag{4·10}$$

Finally (4·7) gives by repeated differentiations

$$(\partial/\partial x)^m(\partial/\partial y)^nF_1(x, y)=w\langle[(\partial/\partial x)+u(\partial/\partial z)]^m[w(\partial/\partial z)]^nF_1(x, z)\rangle$$
$$+u\langle[u(\partial/\partial z)]^m[w(\partial/\partial z)+(\partial/\partial y)]^nF_1(z, y)\rangle, \tag{4·11}$$

which reads more specifically

$$D_2(x, y)=(\partial^2/\partial x\partial y)F_1(x, y)$$
$$=\langle w^2D_2(x, z)+u^2D_2(z, y)\rangle+uw\langle(\partial/\partial z)^2[wF_1(x, z)+uF_1(z, y)]\rangle \tag{4·12}$$

and $$D_3(x, y)=(\partial^2/\partial x\partial y)^2F_1(x, y)=\langle w^3D_3(x, z)+u^3D_3(z, y)\rangle \tag{4·13}$$
$$+2uw\langle(\partial/\partial z)^2[w^2D_2(x, z)+u^2D_2(z, y)]\rangle+(uw)^2\langle(\partial/\partial z)^4[wF_1(x, z)+uF_1(z, y)]\rangle.$$

§ 5. Unitarity of the semi-classical kernel

Before entering into the main subject of the present section to show (1·16), we shall first evaluate the free kernel or the transformation function corresponding to the classical free motion, for which the action function is $S_f(x, y, T)=(m/2T)\times(x-y)^2$. According to the definition (1·9) the semi-classical kernel reads

$$K_f(x, y, T)=(m/2\pi i\hbar T)^{1/2}\exp[(im/2\hbar T)(x-y)^2]$$
$$=(1/2\pi)\int_{-\infty}^{+\infty}du\exp[-(i\hbar T/2m)u^2+iu(x-y)]$$
$$=\exp[(i\hbar T/2m)(\partial/\partial x)^2]\delta(x-y)$$
$$=\exp[-(iT/\hbar)H(p)]\delta(x-y) \tag{5·1}$$

with $H(p)=(1/2m)p^2$ and $p=-i\hbar(\partial/\partial x)$, which is evidently a unitary one. Then we have two equivalent expressions

$$K_f(x, y, T)=\exp[\lambda\mu(\partial/\partial x)^2]\delta(x-y) \tag{5·2}$$

and $$K_f(x, y, T)=\exp[\lambda\mu(\partial/\partial y)^2]\delta(x-y), \tag{5·3}$$

where we have put

$$\lambda=-iT/\hbar,\quad \mu=-\hbar^2/2m \tag{5·4}$$

and accordingly $a=T^2/2m=\lambda^2\mu$.

Proceeding to the general case of an arbitrary potential $V(q)$, the action function is given by

$$S(x, y, T)=S_f(x, y, T)-TF(x, y, T), \tag{2·5}$$

and we have according to (2·6)

$$F(x, y, T)=F_1(x, y)+\lambda^2\mu F_3(x, y)+O(\lambda^4). \tag{5·5}$$

Then since the above (2·5) gives

$$\partial^2S(x, y, T)/\partial x\partial y=-(m/T)[1+(T^2/m)\partial^2F(x, y, T)/\partial x\partial y], \tag{5·6}$$

the semi-classical kernel (1·9) is rewritten according to (5·3) as

$$K_c(x, y, T)=K_f(x, y, T)W(x, y, T)$$
$$=W(x, y, T)\exp[\lambda\mu(\partial/\partial y)^2]\delta(x-y), \tag{5·7}$$

wherein $W(x, y, T)$ is defined according to (5, 5) by

$$\log[W(x, y, T)] = \lambda F(x, y, T) + (1/2)\log[1+2\lambda^2\mu\partial^2 F/\partial x\partial y]$$
$$= \lambda F_1(x, y) + \lambda^2\mu D_2(x, y) + \lambda^3\mu F_3(x, y) + O(\lambda^4). \quad (5\cdot8)$$

We thus get the expansion

$$W(x, y, T) = \sum_{j=0}^{\infty} (\lambda^j/j!)\, W_j(x, y) \quad (5\cdot9)$$

with

$$W_0(x, y) = 1, \quad W_1(x, y) = F_1(x, y),$$
$$W_2(x, y) = F_1(x, y)^2 + 2\mu D_2(x, y), \quad (5\cdot10)$$
$$W_3(x, y) = F_1(x, y)^3 + 6\mu[F_3(x, y) + F_1(x, y)D_2(x, y)].$$

With the aid of the abbreviation $\langle\varphi(x, y)\rangle = \varphi(x, x)$ one accordingly gets by repeated partial integrations

$$\int dy\, K_c(x, y, T)\psi(y) = \int dy\, \delta(x-y)\exp[\lambda\mu(\partial/\partial y)^2]\, W(x, y, T)\psi(y)$$
$$= \sum_{k=0}^{\infty}\sum_{j=0}^{\infty} (1/k!\,j!)(\lambda\mu)^k\lambda^j\langle(\partial/\partial y)^{2k} W_j(x, y)\psi(y)\rangle$$
$$= \sum_{n=0}^{\infty} (\lambda^n/n!) \sum_{k=0}^{n} {}_nC_k\mu^k \sum_{j=0}^{2k} {}_{2k}C_j\langle(\partial/\partial y)^j W_{n-k}(x, y)\rangle (d/dx)^{2k-j}\psi(x), \quad (5\cdot11)$$

which at once yields

$$K_c(x, y, T) = \sum_{n=0}^{\infty} (\lambda^n/n!)\, M_n(x, \partial/\partial x)\,\delta(x-y) \quad (5\cdot12)$$

with the differential operators

$$M_n(x, \partial/\partial x) = [\mu(\partial/\partial x)^2]^n$$
$$+ \sum_{k=0}^{n-1} {}_nC_k\mu^k \sum_{j=0}^{2k} {}_{2k}C_j\langle(\partial/\partial y)^j W_{n-k}(x, y)\rangle(\partial/\partial x)^{2k-j}. \quad (5\cdot13)$$

Since (1·15), (2·14) and (4·12) furnish the relationships

$$\langle(\partial/\partial y)^n F_1(x, y)\rangle = (n+1)^{-1} V_n(x),$$
$$\langle(\partial/\partial y) F_1(x, y)^2\rangle = V(x)\, V_1(x),$$
$$\langle(\partial/\partial y)^2 F_1(x, y)^2\rangle = (2/3)\, V(x)\, V_2(x) + (1/2)\, V_1(x)^2, \quad (5\cdot14)$$
$$\langle F_3(x, y)\rangle = (1/12)\, V_1(x)^2,$$
$$\langle(\partial/\partial y)^n D_2(x, y)\rangle = [(n+2)(n+3)]^{-1} V_{n+2}(x),$$

we have according to (5·10)

$$\langle(\partial/\partial y)^n W_1(x, y)\rangle = (n+1)^{-1} V_n(x),$$
$$\langle W_2(x, y)\rangle = V(x)^2 + (\mu/3)\, V_2(x),$$

$$\langle(\partial/\partial y)\,W_2(x,\,y)\rangle = V(x)\,V_1(x) + (\mu/6)\,V_3(x), \tag{5·15}$$

$$\langle(\partial/\partial y)^2W_2(x,\,y)\rangle = (2/3)\,V(x)\,V_2(x) + (1/2)\,V_1(x)^2 + (\mu/10)\,V_4(x),$$

$$\langle W_3(x,\,y)\rangle = V(x)^3 + \mu[(1/2)\,V_1(x)^2 + V(x)\,V_2(x)].$$

One obtains, therefore, from (5·13) the results: $M_0(x,\,\partial/\partial x) = 1$,

$$M_1(x,\,\partial/\partial x) = \mu(\partial/\partial x)^2 + \langle W_1(x,\,y)\rangle = \mu(\partial/\partial x)^2 + V(x), \tag{5·16}$$

$$\begin{aligned} M_2(x,\,\partial/\partial x) &= \mu^2(\partial/\partial x)^4 + 2\mu[\langle(\partial/\partial y)^2W_1\rangle + 2\langle(\partial/\partial y)\,W_1\rangle(\partial/\partial x) \\ &\qquad + \langle W_1\rangle(\partial/\partial x)^2] + \langle W_2\rangle \\ &= \mu^2(\partial/\partial x)^4 + \mu[V_2 + 2V_1(\partial/\partial x) + 2V(\partial/\partial x)^2] + V^2 \\ &= [\mu(\partial/\partial x)^2 + V(x)]^2, \end{aligned} \tag{5·17}$$

$$\begin{aligned} M_3(x,\,\partial/\partial x) &= \mu^3(\partial/\partial x)^6 + \mu^2[(9/10)\,V_4 + 4V_3(\partial/\partial x) + 7V_2(\partial/\partial x)^2 \\ &\qquad + 6V_1(\partial/\partial x)^3 + 3V(\partial/\partial x)^4] \\ &\quad + \mu[3VV_2 + 2V_1^2 + 6VV_1(\partial/\partial x) + 3V^2(\partial/\partial x)^2] + V^3 \\ &= [\mu(\partial/\partial x)^2 + V(x)]^3 - (\mu^2/10)\,V_4(x). \end{aligned} \tag{5·18}$$

Therefore, (5·4) and (1·5) tell us that the above (5·12) is identical with (1·16) up to the terms of the third order in T.

Only when $V_4(x)$ vanishes, it is thus possible that the semi-classical kernel is a unitary one. It will then be shown for the classical potential $V(q)$ given by (2·2) that the corresponding $K_c(x,\,y,\,T)$ is identical with the transformation function (1·3), or more precisely that

$$K_c(x,\,y,\,T) = \exp[\lambda\mu(\partial/\partial x)^2 + \lambda V(x)]\,\delta(x-y). \tag{5·19}$$

For the linear potential $V(q) = kq$ we have according to (2·3), (5·2) and (5·4)

$$\begin{aligned} K_c(x,\,y,\,T) &= \exp[(\lambda k/2)\,(x+y) + (1/12)\,\lambda^3\mu k^2]\cdot K_f(x,\,y,\,T) \\ &= \exp(\lambda^3\mu k^2/12)\exp(\lambda kx/2)\exp[\lambda\mu(\partial/\partial x)^2]\exp(\lambda kx/2)\,\delta(x-y). \end{aligned} \tag{5·20}$$

This is transformed into (5·19) by putting $u = \lambda\mu$ and $w = k/2\mu$ in Equation (A·1) in the Appendix. Then for the quadratic potential $V(q) = (m\omega^2/2)\,q^2$ the classical action (2·4) is rewritten with $\omega T^* = \sin\omega T$ as

$$S(x,\,y,\,T) = S_f(x,\,y,\,T^*) - (m\omega/2)\,(x^2+y^2)\tan(\omega T/2), \tag{5·21}$$

so that one has by putting $u = \omega T/2$ and $w = i\hbar/m\omega$

$$\begin{aligned} K_c(x,\,y,\,T) &= \exp[(m\omega/2i\hbar)\,(x^2+y^2)\tan(\omega T/2)]\cdot K_f(x,\,y,\,T^*) \\ &= \exp[(1/2w)\,x^2\tan u]\exp[(w/2)\sin 2u\,(\partial/\partial x)^2]\exp[(1/2w)x^2\tan u]\,\delta(x-y). \end{aligned} \tag{5·22}$$

Then since $uw = \lambda\mu$ and $u/w = \lambda(m\omega^2/2)$, the identity (A·2) again yields the above (5·19). This furnishes an improvement of the operator calculus that was given in 1952 by the author.[8)]

§ 6. Solution of the integral equation

The function $U(x, y, T)$ in $(1\cdot 21)$ is rewritten according to $(5\cdot 4)$ as

$$U(x, y, T)=1+(1/2)\lambda^3\mu^2 D(x, y)+O(\lambda^4) \tag{6·1}$$

and we have from $(1\cdot 19)$ and $(5\cdot 8)$

$$K(x, y, T)=K_c(x, y, T)U(x, y, T)=K_f(x, y, T)Y(x, y, T) \tag{6·2}$$

with

$$Y(x, y, T)=W(x, y, T)U(x, y, T). \tag{6·3}$$

Then since $(4\cdot 4)$ gives with $w=1-u$ and $g(u)=ux+wy$

$$K_f(x, z, wT)K_f(z, y, uT)=K_f(x, y, T)K_f[z, g(u), uwT], \tag{6·4}$$

the integral equation $(1\cdot 23)$ is transformed into

$$\begin{aligned} K(x, y, T)&=\int K(x, z, wT)\,dz\,K(z, y, uT)\\ &=K_f(x, y, T)\int dz\,K_f[z, g(u), uwT]\,Y(x, z, wT)\,Y(z, y, uT)\\ &=K(x, y, T)\int dz\,\delta[z-g(u)]\exp[\lambda\mu\,uw(\partial/\partial z)^2]\\ &\qquad\times Y(x, z, wT)\,Y(z, y, uT)\,Y(x, y, T)^{-1}. \end{aligned} \tag{6·5}$$

In terms of the symbol $\langle\varphi(x, y, z)\rangle=\varphi[x, y, g(u)]$ we thus get the equation

$$1=\langle\exp[\lambda\mu\,uw(\partial/\partial z)^2]\,Y(x, z, wT)\,Y(z, y, uT)\,Y(x, y, T)^{-1}\rangle. \tag{6·6}$$

By putting

$$Y_1(x, y, z)=wF_1(x, z)+uF_1(z, y)-F_1(x, y) \tag{6·7}$$

we get from $(5\cdot 8)$

$$\begin{aligned} &\log[W(x, z, wT)\,W(z, y, uT)\,W(x, y, T)^{-1}]=\lambda Y_1(x, y, z)\\ &+\lambda^2\mu[w^2D_2(x, z)+u^2D_2(z, y)-D_2(x, y)]\\ &+\lambda^3\mu[w^3F_3(x, z)+u^3F_3(z, y)-F_3(x, y)]+O(\lambda^4), \end{aligned} \tag{6·8}$$

which yields together with the above $(6\cdot 1)$

$$Y(x, z, wT)\,Y(z, y, uT)\,Y(x, y, T)^{-1}=\sum_{j=0}^{\infty}(\lambda^j/j!)\,Y_j(x, y, z) \tag{6·9}$$

with $Y_0(x, y, z)=1$ and

$$Y_2(x, y, z)=Y_1(x, y, z)^2+2\mu[w^2D_2(x, z)+u^2D_2(z, y)-D_2(x, y)], \tag{6·10}$$

$$\begin{aligned} Y_3(x, y, z)&=Y_1(x, y, z)^3+6\mu[w^3F_3(x, z)+u^3F_3(z, y)-F_3(x, y)]\\ &\quad+6\mu Y_1(x, y, z)\cdot[w^2D_2(x, z)+u^2D_2(z, y)-D_2(x, y)]\\ &\quad+3\mu^2[w^3D(x, z)+u^3D(z, y)-D(x, y)]. \end{aligned} \tag{6·11}$$

Then we have according to $(4\cdot 7)$, $(4\cdot 12)$ and $(4\cdot 10)$ the relationships

$$\langle Y_1(x, y, z)\rangle = 0,$$
$$\langle Y_2(x, y, z)\rangle = -2\mu uw\langle(\partial/\partial z)^2 Y_1(x, y, z)\rangle, \tag{6·12}$$
$$\langle Y_3(x, y, z)\rangle - 3\mu^2[\langle w^3 D(x, z) + u^3 D(z, y)\rangle - D(x, y)]$$
$$= -6\mu uw\langle(\partial/\partial z) Y_1(x, y, z)\rangle^2 = -3\mu uw\langle(\partial/\partial z)^2 Y_1(x, y, z)^2\rangle,$$

so that the above (6·6) and (6·9) give

$$0 = \sum_{k=0}^{\infty}\sum_{j=0}^{\infty}(1/k!\,j!)\lambda^{k+j}(\mu uw)^k\langle(\partial/\partial z)^{2k} Y_j(x, y, z)\rangle - 1$$
$$= \sum_{n=1}^{\infty}(\lambda^n/n!)\sum_{k=0}^{n-1}{}_nC_k(\mu uw)^k\langle(\partial/\partial z)^{2k} Y_{n-k}(x, y, z)\rangle$$
$$= \lambda\langle Y_1\rangle + (\lambda^2/2)[\langle Y_2\rangle + 2\mu uw\langle(\partial/\partial z)^2 Y_1\rangle]$$
$$+ (\lambda^3/6)[\langle Y_3\rangle + 3\mu uw\langle(\partial/\partial z)^2 Y_2\rangle + 3(\mu uw)^2\langle(\partial/\partial z)^4 Y_1\rangle] + O(\lambda^4)$$
$$= (\lambda^3\mu^2/2)[\langle w^3 D(x, z) + u^3 D(z, y)\rangle - D(x, y)$$
$$+ (uw/\mu)\langle(\partial/\partial z)^2(Y_2 - Y_1^2)\rangle + (uw)^2\langle(\partial/\partial z)^4 Y_1\rangle] + O(\lambda^4). \tag{6·13}$$

Therefore the equation for determining the function $D(x, y)$ is

$$D(x, y) = \langle w^3 D(x, z) + u^3 D(z, y)\rangle$$
$$+ 2uw\langle(\partial/\partial z)^2[w^2 D_2(x, z) + u^2 D_2(z, y)]\rangle$$
$$+ (uw)^2\langle(\partial/\partial z)^4[wF_1(x, z) + uF_1(z, y)]\rangle, \tag{6·14}$$

which is identical in structure with (4·13). We thus get the solution (1·24).

§ 7. Quantization of the Lagrangian $L = (m/2)[w(q)v]^2$

If the classical Lagrangian is of the form

$$L(q, v) = L(R) \quad \text{with} \quad R = w(q)\, dq/dt \tag{7·1}$$

and d^2L/dR^2 does not vanish, the Lagrangian equation of motion (1·7) gives $dR/dt = 0$, which is integrated at once to give

$$R = (1/T)\int_y^x dq\, w(q)\,. \tag{7·2}$$

When the Lagrangian is quadratic in R, as is given in (1·26), we get the classical action

$$S(x, y, T) = T(m/2)R^2 = (m/2T)\Big[\int_y^x dq\, w(q)\Big]^2$$
$$= (m/2T)(X - Y)^2 = S_f(X, Y, T) \tag{7·3}$$

with $X = \int_0^x dq w(q)$ and $Y = \int_0^y dq w(q)$. Then since

$$\partial^2 S(x, y, T)/\partial x \partial y = -(m/T) w(x) w(y), \tag{7·4}$$

the semi-classical kernel (1·9) reads

$$K_c(x, y, T) = [w(x) w(y)]^{1/2} K_f(X, Y, T), \tag{7·5}$$

which gives for $T=0$

$$K_c(x, y, 0) = [w(x) w(y)]^{1/2} \delta(X-Y) = \delta(x-y). \tag{7·6}$$

Now putting $G(u) = uX + wY$ with $w = 1-u$, we get according to (6·4)

$$K_f(X, Z, wT) K_f(Z, Y, uT) = K_f(X, Y, T) K_f[Z, G(u), uwT] \tag{7·7}$$

and then putting $Z = \int_0^z dq\, w(q)$ with $dZ = w(z) dz$, (7·5) and the relationship $\int dZ K_f[Z, G(u), uwT] = 1$ give at once

$$\int K_c(x, z, wT)\, dz\, K_c(z, y, uT) = K_c(x, y, T). \tag{7·8}$$

The semi-classical kernel $K_c(x, y, T)$ can thus be identified with the unitary transformation function $K(x, y, T)$.

According to (5·1) we get the integral representation

$$K(x, y, T) = (1/2\pi)[w(x) w(y)]^{1/2} \int dk \exp[-(iT/\hbar)(\hbar^2 k^2/2m) + ik(X-Y)], \tag{7·9}$$

which is nothing but the eigenfunction expansion of the transformation function and accordingly the normalized orthogonal eigenfunction $\psi_k(x)$ corresponding to the energy eigenvalue $E = \hbar^2 k^2/2m$ is

$$\psi_k(x) = [w(x)/2\pi]^{1/2} \exp[ik \int_0^x dq\, w(q)]. \tag{7·10}$$

Since this satisfies the equation

$$w(x)^{-1/2} \cdot p \cdot w(x)^{-1/2} \psi_k(x) = \hbar k \psi_k(x) \tag{7·11}$$

with $p = -i\hbar(d/dx)$, the Hamiltonian operator for this system is

$$H(x, p) = (1/2m)[w(x)^{-1/2} \cdot p \cdot w(x)^{-1/2}]^2. \tag{7·12}$$

Appendix

In this appendix we shall establish the identities

$$\exp[u(d/dx)^2 + 2uwx] = \exp(uwx) \exp[u(d/dx)^2] \exp(uwx) \exp[(1/3) u^3 w^2] \tag{A·1}$$

and

$$\exp[uw(d/dx)^2 + (u/w) x^2] = \exp[(1/2w) x^2 \tan u] \times \exp[(w/2) \sin 2u (d/dx)^2] \cdot \exp[(1/2w) x^2 \tan u]. \tag{A·2}$$

In order to prove (A·1) we first put its right-hand side in the form

$$=\exp[f(u)wx]\exp[g(u)(d/dx)^2]\exp[f(u)wx]\exp[w^2h(u)]$$

with the unknown functions $f(u)$, $g(u)$ and $h(u)$ in the parameter u, for which we must put $f(0)=g(0)=h(0)=0$. Then the differentiation of both sides with respect to u gives

$$\begin{aligned}(d/dx)^2+2wx=&f'(u)wx+g'(u)e^{f(u)wx}(d/dx)^2e^{-f(u)wx}\\&+f'(u)w\cdot e^{f(u)wx}e^{g(u)(d/dx)^2}\cdot x\cdot e^{-g(u)(d/dx)^2}e^{-f(u)wx}+w^2h'(u)\\&=f'(u)wx+g'(u)[(d/dx)-f(u)w]^2\\&+f'(u)w[x+2g(u)[(d/dx)-f(u)w]]+w^2h'(u),\end{aligned}$$

which at once yields $f'(u)=g'(u)=1$. So we have $f(u)=g(u)=u$ and $h'(u)=u^2$. Then we get $h(u)=(1/3)u^3$ and accordingly (A·1) is proved. The (A·2) can be established in quite the same way, so the proof is omitted here.

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