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Semiclassical approximation in the Weyl picture by path summation

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Abstract. Quantum mechanics may be formulated in pseudo-phasespace in the Weyl picture. The semiclassical expression for the Weyl transform of the usual time evolution operator is evaluated by summing over paths a semiclassical approximation for a new propagator in pseudo-phasespace. As an example the Bohr-Sommerfeld quantisation rule is recovered. The new propagator may in principle be used to construct other interesting quantities, such as the propagator governing the time evolution of the Wigner function.

1. Introduction

The usual formation of quantum mechanics in terms of operators on a Hilbert space has, by means of the Weyl picture, a completely equivalent expression in terms of functions defined on what might be termed a pseudo-phasespace (p, q) (Weyl 1927, 1931, Wigner 1932, Moyal 1949, Imre *et al* 1967, Leaf 1968a, b). But the formulation seems generally to encourage only wide ranging non-specific analyses of the interface between classical mechanics and quantum mechanics. A notable recent exception to this is a paper by Berry (1977), who exhibits in the Weyl picture the form of a quantum pure state in both the usual semiclassical and uniform approximations.

In the present paper we derive the semiclassical approximation, in the Weyl picture, for the time evolution operator (§ 5) by defining a new propagator (§ 4) appropriate to the pseudo-phasespace of the Wigner–Weyl picture (§ 2). This new propagator bears some similarity to the usual propagator $\langle xt|x'0\rangle$ of quantum mechanics and may be summed over paths. Indeed, the well known results of semiclassical path sums on $\langle xt|x'0\rangle$ outlined in § 3 may be taken over formally to pseudo-phasespace. In § 6 we briefly consider the Bohr–Sommerfeld quantisation rule from the standpoint of pseudo-phasespace. Possible future applications of the Weyl picture to semiclassical approximations are suggested in § 7.

2. The Wigner–Weyl picture

Throughout this paper we assume that the pseudo-phasespace formulation is fairly well known. In any case, thorough discussions are given in many references. An easily read general treatment is given by de Groot and Suttorp (1972). Papers by Moyal (1949), Leaf (1968a, b) and Imre *et al* (1967) also provide a general view.

The Weyl transform relating any operator A to its Weyl equivalent $A(pq)$ may be written

$$A(p,q)=\mathrm{Tr}(A\Delta(p,q)) \tag{1}$$

$$A=\int\frac{\mathrm{d}p\,\mathrm{d}q}{h}A(p,q)\Delta(p,q) \tag{2}$$

where the Hermitian operator Δ is given formally by

$$\Delta(p,q)=\int \mathrm{d}x\,\exp\left(\frac{\mathrm{i}}{\hbar}px\right)\left|q+\frac{x}{2}\right\rangle\left\langle q-\frac{x}{2}\right|. \tag{3}$$

Throughout we shall work for simplicity in one dimension.

A special case is the Wigner function (Wigner 1932) $\rho(pqt)$ which may be defined as the Weyl transform of the density matrix ρ_t. The time propagation of the Wigner function is briefly considered in §§ 4 and 7.

Two properties of the operator Δ which we shall need are

$$\int\frac{\mathrm{d}p\,\mathrm{d}q}{h}\Delta(pq)=1 \tag{4}$$

$$\mathrm{Tr}(\Delta(pq)\Delta(p_0q_0))=h\delta(p-p_0)\delta(q-q_0). \tag{5}$$

Now part of the attraction of this picture of quantum mechanics is that it sometimes has a classical 'look' to it. For example, one can show that the trace of the product of two operators takes the following form:

$$\mathrm{Tr}(AB)=\int(\mathrm{d}p\,\mathrm{d}q/h)A(pq)B(pq). \tag{6}$$

Thus, since the Weyl transform of the unit operator is unity, we have for the density matrix

$$\mathrm{Tr}\,\rho_t=\int\frac{\mathrm{d}p\,\mathrm{d}q}{h}\rho(pqt).$$

The Weyl picture is of course fully quantum. For example, the Weyl transform of the product AB of two operators is not the product of the seperate Weyl transforms, but is given by

$$(AB)(pq)=A(pq)\exp\left[\frac{\mathrm{i}\hbar}{2}\left(\frac{\partial^*}{\partial q}\frac{\partial}{\partial p}-\frac{\partial^*}{\partial p}\frac{\partial}{\partial q}\right)\right]B(pq). \tag{7}$$

Here the starred operators act to the *left* on $A(pq)$ only.

3. The usual semiclassical path summation

In the customary formulation of quantum mechanics by path summation (Feynman and Hibbs 1965) one works with the propagator

$$\langle xt|x'0\rangle=\langle x|U_t|x'\rangle.$$

By splitting the interval $(0,t)$ into a large number of subintervals Δt, one may express the propagator as a sum over paths in position. In particular we may write

$$\psi(xt)=\int \mathrm{d}x'\ldots \mathrm{d}x''\langle xt|x't-\Delta t\rangle\langle x't-\Delta t|\ldots\rangle\langle x''0|\psi_0\rangle \tag{8}$$

where the initial state is

$$\psi(x,0)=\langle x0|\psi_0\rangle.$$

In the customary semiclassical approximation one obtains a semiclassical approximation for the short-time propagator $\langle xt|x't-\Delta t\rangle$ and then performs the path sum (8) in the sense of stationary phase (Berry and Mount 1972).

If we consider an n-dimensional system x_i, where $i=1,2,\ldots n$, then the short-time semiclassical propagator is (Van Vleck 1928, Berry and Mount 1972, Maslov 1962)

$$\langle xt|x'0\rangle\simeq\left[\frac{1}{(2\pi i\hbar)^{1/2}}\right]^n\left(\left|\det\frac{\partial^2 S}{\partial x_i\,\partial x_j'}\right|\right)^{1/2}\exp[(i/\hbar)S(xt|x'0)]. \tag{9}$$

Here S is the action, calculated for classical motion according to Hamilton's equations, and considered as a function of x, x' and t.

In the process of using approximation (9) to obtain a semiclassical approximation for $\psi(x,t)$ in the sense of stationary phase, one needs to take care at focal points (caustics). This has been considered with considerable mathematical honesty by Maslov (1962) and we now briefly summarise the relevant results.

For a Hamiltonian

$$\sum_i \tfrac{1}{2}p_i^2+V(x_1,x_2\ldots x_n)$$

the final state becomes, in the semiclassical approximation (theorem 1.1 of Maslov's paper),

$$\psi(x,t)\simeq\sum_k \psi(x_0^{(k)},0)\frac{\exp\{(i/\hbar)[S(xt|x_0^{(k)}0)-(\hbar/2)m(x_0^{(k)},t)]\}}{(|\det\partial X_i(x_0^{(k)},t)/\partial x_{0j}|)^{1/2}}. \tag{10}$$

In this expression the initial state is assumed to have the form

$$\psi(x,0)=\phi(x)\exp(i/\hbar)f(x). \tag{11}$$

The process $X_i(x_0^{(k)},t)$ is a solution to Hamilton's equations with initial conditions

$$X_i(t=0)=x_{0i} \tag{12a}$$

$$\dot X_i(t=0)=\mathrm{grad}_i f(x_0) \tag{12b}$$

and the initial value x_0 is chosen so that (for given t and x)

$$X_i(x_0^{(k)},t)=x_i. \tag{13}$$

Since there may be more than one initial position x_0 satisfying this equation, we label them by a superscript k, thus $x_0^{(k)}$. Equation (13) thus determines the initial values $x_0^{(k)}$ as a function of given values of x and t.

In equation (10) the action S is calculated for the process $X_i(x_0^{(k)},\tau)$ with $t\geqslant\tau\geqslant 0$ and the phases m are the contributions of the focal points to the kth classical path $X(x_0^{(k)},\tau)$. Focal points are those points along the trajectory such that the determinant in the denominator of equation (10) vanishes. The index m of the kth classical path is the sum of all the foci lying on this path where the index of a particular focus is $(n-\sigma)/2$; here n is the dimension of the problem and σ is the signature (number of positive minus number of negative eigenvalues) of the matrix

$$\lim_{\epsilon\to 0} \mathbf{M}(t'+\epsilon) \,.\, \mathbf{M}^{-1}(t'-\epsilon)$$

where the focus occurs at time t' along the path and the matrix $\mathbf{M}$ is given by

$$\mathbf{M}_{ij}(x_0, t) = \partial X_i(x_0, t)/\partial x_{0j}. \tag{14}$$

In § 4 we shall calculate a path summation scheme in the Wigner–Weyl picture that will allow us to adapt these results to find in § 5 a semiclassical approximation for the Weyl transform of the time evolution operator U_t.

4. Propagators in pseudo-phasespace

Particularising to time-independent Hamiltonians, the time evolution operator in Hilbert space is

$$U_t = \exp[(-\mathrm{i}/\hbar)Ht]. \tag{15}$$

By means of this and the Hermitian operator Δ, it is possible to construct a propagator in pseudo-phasespace that takes an initial state represented by the density matrix ρ_0 to its evolved state ρ_t at subsequent times t. Writing this well known propagator as $P(pqt|p_0q_0t_0)$ we have (Leaf 1968a, b, de Groot and Suttorp 1972)

$$\rho(pqt) = \int \mathrm{d}p_0\, \mathrm{d}q_0\, P(pqt|p_0q_0t_0)\rho(p_0q_0t_0). \tag{16}$$

This is the equivalent expression, in the Wigner–Weyl picture, to the time evolution in Hilbert space

$$\rho_t = U_{t-t_0}\rho_0 U^{\dagger}_{t-t_0}.$$

The details are clearly set down in de Groot and Suttorp's book. The propagator P is defined as

$$P(pqt|p_0q_0t_0) = h^{-1}\,\mathrm{Tr}\{U^{\dagger}_{t-t_0}\Delta(pq)U_{t-t_0}\Delta(p_0q_0)\}. \tag{17}$$

Using this definition together with equations (1) and (6), one may show that P obeys the 'Markov property' consistent with a path summation formulation:

$$P(pqt|p_0q_0t_0) = \int \mathrm{d}p_1\, \mathrm{d}q_1\, P(pqt|p_1q_1t_1)P(p_1q_1t_1|p_0q_0t_0). \tag{18}$$

Two further properties of P are noteworthy. They are

$$\lim_{t-t_0\to 0} P(pqt|p_0q_0t_0) = \delta(p-p_0)\delta(q-q_0) \tag{19}$$

$$\int \mathrm{d}p\, \mathrm{d}q\, P(pqt|p_0q_0t_0) = 1. \tag{20}$$

It is our object in this paper to follow in pseudo-phasespace the time evolution, not of states ρ_t, but rather of the propagator U_t itself; we wish to propagate the initial

Weyl transform $U(pqt_0)$ to later times t. For this we now define a new propagator in pseudo-phasespace and give several of its properties. The new propagator is denoted Q, where

$$Q(pqt|p_0q_0t_0) = h^{-1}\,\mathrm{Tr}\{\Delta(pq)U_{(t-t_0)/2}\Delta(p_0q_0)U_{(t-t_0)/2}\} \tag{21}$$

and U_t is given by equation (15).

We may obtain the Weyl transform of U_t by integrating Q over p_0q_0; using equations (4) and (1) it follows (setting $t_0 = 0$ for convenience) that

$$U(pqt) = \int \mathrm{d}p_0\,\mathrm{d}q_0\,Q(pqt|p_0q_00). \tag{22}$$

Furthermore, by using equation (6) it follows that Q satisfies the Markov property (equation (18)) with P replaced by Q. That Q assumes the initial value $\delta(p-p_0)\delta(q-q_0)$ can easily be shown using equation (5).

Q is then a suitable candidate for a path summation; one may find an approximate Q for short times and then construct the long-time propagator by summing paths. This is described in the next section, and explicitly set down, in the semiclassical limit. There we shall need the equation of motion obeyed by Q. This we now find.

Setting $t_0 = 0$ for convenience we have

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}(U_{t/2}\Delta(p_0q_0)U_{t/2}) = \tfrac{1}{2}\{H,\,U_{t/2}\Delta(p_0q_0)U_{t/2}\}$$

where the curly brackets indicate the anticommutator, and we have made use of the fact that H is time-independent and so commutes with U at all times.

Taking the Weyl transform of both sides of this equation (using equation (7)) gives

$$\mathrm{i}\hbar\frac{\partial}{\partial t}Q(pqt|p_0q_00) = L_{pq}Q(pqt|p_0q_00) \tag{23}$$

where the linear operator L is defined by

$$L_{pq}Q = \frac{1}{2}H(pq)\left\{\exp\frac{\mathrm{i}\hbar}{2}\left(\frac{\partial^*}{\partial q}\frac{\partial}{\partial p} - \frac{\partial^*}{\partial p}\frac{\partial}{\partial q}\right) + \mathrm{cc}\right\}Q \tag{24}$$

where $\partial^*/\partial p$ and $\partial^*/\partial q$ operate *to the left* on $H(pq)$, the Weyl transform of the Hamiltonian H.

5. Semiclassical path sum in pseudo-phasespace

In order to extend the results outlined in § 3 to obtain a semiclassical approximation in pseudo-phasespace, we must first find a short-time approximation for Q corresponding to the Van Vleck expression (9). To do this we mimick the method of van Vleck (1928) outlined by Mizrahi (1977), as it applies to the Wigner–Weyl picture.

To find a semiclassical approximation for the new propagator Q we seek a solution to equation (23) in the form

$$Q = C(pqt)\exp[(\mathrm{i}/\hbar)\mathrm{D}(pqt)]. \tag{25}$$

We have in this way extracted the non-analytical behaviour at the origin, $\hbar = 0$, hoping that D will have a well defined expansion in powers of $\hbar$:

$$D = a + \hbar^2 b + \dots .$$

The function D is also assumed to be real-valued.

To obtain equations of motion for C and a we replace the exact equation (23) by an equation correct to order $\hbar^2$. That is, we require that the left-hand side of the exact equation

$$Q^{-1}[\mathrm{i}\hbar(\partial/\partial t) - L_{pq}]Q = 0$$

vanishes to orders zero and one in powers of $\hbar$. Inserting the assumed form (25) for Q gives two equations of motion for C and a by equating to zero the coefficients of the zero and first-order powers of $\hbar$.

The algebra leading to these equations is fairly complicated but straightforward. Assuming a Hamiltonian of the form

$$H(pq) = (p^2/2m) + V(q) \tag{26}$$

one finds that the equation resulting by equating the coefficient of the zero power of $\hbar$ to zero is

$$0 = \frac{\partial a}{\partial t} + \frac{1}{2}\left(H\left(p + \frac{1}{2}\frac{\partial a}{\partial q}, q - \frac{1}{2}\frac{\partial a}{\partial p}\right) + H\left(p - \frac{1}{2}\frac{\partial a}{\partial q}, q + \frac{1}{2}\frac{\partial q}{\partial p}\right)\right). \tag{27}$$

This is a Hamilton–Jacobi equation with generalised *two-dimensional* Hamiltonian $\mathcal{H}$

$$\mathcal{H}(p_1 p_2 x_1 x_2) = \frac{1}{2m}\left[(x_1)^2 + \left(\frac{p_2}{2}\right)^2\right] + \tfrac{1}{2}[V(x_2 - \tfrac{1}{2}p_1) + V(x_2 + \tfrac{1}{2}p_1)] \tag{28}$$

where the generalised coordinates are $(x_1 x_2) \leftrightarrow (p, q)$ and corresponding momenta are

$$(p_1, p_2) \leftrightarrow \left(\frac{\partial a}{\partial p}, \frac{\partial a}{\partial q}\right).$$

Equating to zero the coefficient of the first power of $\hbar$, we obtain the 'equation of continuity' for C^2:

$$0 = \frac{\partial}{\partial t} C^2 + \frac{\partial}{\partial p}\left\{C^2\left[\frac{\partial}{\partial p_1}\mathcal{H}(pqp_1p_2)\right]_{p_1 = \partial a/\partial p,\, p_2 = \partial a/\partial q}\right\}$$
$$+ \frac{\partial}{\partial q}\left\{C^2\left[\frac{\partial}{\partial p_2}\mathcal{H}(pqp_1p_2)\right]_{p_1 = \partial a/\partial p,\, p_2 = \partial a/\partial q}\right\}. \tag{29}$$

The relevant formal solutions to equations like (27) and (29) are well known (Van Vleck 1928, Schiller 1962). We have

$$a = S(xt|x'0) \tag{30}$$

where S is the action calculated for the classical trajectory connecting points (x_1, x_2) and (x_1', x_2') in time t (for small time t there will only be one such trajectory). For the quantity C we have

$$C = \text{const.}\,(\det \partial^2 a/\partial x_i\, \partial x_j')^{1/2}. \tag{31}$$

Here the constant factor takes into account the arbitrary choice of phase and initial condition (19).

As a parenthetical comment we note that it is well known that semiclassical approximations such as (10) or (25), (30) and (31) are *exact* for Hamiltonians at most quadratic in p and q.

Thus, for a harmonic oscillator

$$H(pq)=\frac{p^2}{2m}+\frac{1}{2}m\omega^2q^2$$

and one may show that the *exact* propagator Q is given by

$$Q(x_1x_2t|x'_1x'_20)$$
$$=\left(\frac{\mathrm{i}}{2\pi\hbar}\right)^{1/2}\frac{2}{\sin(\omega t/2)}\exp[\![(\mathrm{i}/\hbar)(1/m\omega\sin(\omega t/2))$$
$$\times\{[(x_1^2+m^2\omega^2x_2^2)\cos(\omega t/2)-(x_1x'_1+m^2\omega^2x_2x'_2)]+[x\leftrightarrow x']\}]\!].$$

Now, according to equations (22) and (18) (for Q), we may adapt the results obtained in § 3 to obtain a semiclassical approximation for $U(pqt)$ provided we replace the initial state $\psi(x, 0)$ by unity. Thus in equation (11) we must choose $\phi=1$ and $f(x)=0$. The sum is now over variables $(x_1, x_2)\leftrightarrow(p, q)$.

Since we are here working with a Hamiltonian $\mathscr{H}$ that is not of the form (26), we must take into account the fact that the generalised momenta p_i are not the same as $\dot{x}_i$. A careful look at Maslov's treatment, for instance, shows that initial conditions (12) must be replaced by

$$X_i(t=0)=x_{0i} \tag{33a}$$

$$P_i(t=0)=0 \tag{33b}$$

where P_i and X_i is the classical process in four-dimensional phasespace, with the Hamiltonian $\mathscr{H}$ given by equation (28).

In general, the process $X_i(t)$ is actually simply related to two one-dimensional systems. The Hamilton equations for X and P are

$$\dot{X}_1=-\tfrac{1}{4}(V'(X_2-\tfrac{1}{2}P_1)-V'(X_2+\tfrac{1}{2}P_1)) \tag{34a}$$

$$\dot{P}_1=(-1/m)X_1 \tag{34b}$$

$$\dot{X}_2=(1/4m)P_2 \tag{34c}$$

$$\dot{P}_2=-\tfrac{1}{2}(V'(X_2-\tfrac{1}{2}P_1)+V'(X_2+\tfrac{1}{2}P_1)). \tag{34d}$$

If we now define new quantities

$$Q^{\pm}=X_2\pm\tfrac{1}{2}P_1 \tag{35a}$$

$$P^{\pm}=4m\dot{Q}^{\pm} \tag{35b}$$

it then follows from equations (34) that

$$\dot{P}^{\pm}=-V'(Q^{\pm}) \tag{35c}$$

$$P^{\pm}=P_2\mp2X_1. \tag{35d}$$

We now see that the plus and minus systems move independently of one another according to Newton's law. Thus there are in general *two* independent constants of the motion corresponding to the energy of the two systems. According to equation

(35b), where the 'mass' is $4m$, we have the following two constants of the motion:

$$E^{\pm} = (1/8m)(P^{\pm})^2 + V(Q^{\pm}). \tag{36}$$

Thus the system (34) is integrable.

We also note that the full Hamiltonian $\mathscr{H}$ is a constant of motion and is given by

$$\mathscr{H} = \tfrac{1}{2}(E^+ + E^-). \tag{37}$$

Now initial conditions (33) must be met. In particular, the initial momenta P_i must vanish. The implications of this for the plus and minus systems follows from equations (35a) and (35d). We have

$$Q^+(0) = Q^-(0) \tag{38a}$$

$$P^+(0) = -P^-(0). \tag{38b}$$

It is then clear, in this special case, that the constants E^+ and E^- become equal to each other and to $\mathscr{H}$.

We may express the action for the process (34) in terms of the plus and minus systems. We have (integrating by parts on X_1),

$$\int_0^t \mathrm{d}s \left(\sum_i P_i(s)\dot{X}_i(s) - \mathscr{H}\right)$$

$$= [P_1X_1]_0^t + \int_0^t \mathrm{d}s \left(\frac{P_2^2}{4m} + \frac{X_1^2}{m}\right) - \mathscr{H}t.$$

Expressing P_2 and X_1 in terms of $P^{\pm}$ by means of equation (35d) and utilising equation (37) gives

$$\int_0^t \mathrm{d}s \left(\sum_i P_i\dot{X}_i - \mathscr{H}\right)$$

$$= [P_1X_1]_0^t + \frac{1}{2}\left[\int_0^t \mathrm{d}s \left(\frac{P^{+2}}{4m} - E^+\right) + \int_0^t \mathrm{d}s \left(\frac{P^{-2}}{4m} - E^-\right)\right]. \tag{39}$$

One recognises the last two terms in square brackets as the usual action for the plus and minus systems for a mass $4m$ under the force $-V'(Q^{\pm})$.

Finally, we must consider the contributions of focal points to the phase $-(\pi/2)m(x_0^{(k)}, t)$. We must examine those times t' such that $\det \mathbf{M}(t') = 0$, under the conditions $P_i(0) = 0$, where the two-by-two matrix $\mathbf{M}$ is given by equation (14). Let us define $Q^+(0) = Q_0$ and $P^+(0) = P_0$. Then from equations (35a) and (35d) we have $X_1 = \frac{1}{4}(P^- - P^+)$ and $X_2 = \frac{1}{2}(Q^+ + Q^-)$. Thus $x_{01} = -\frac{1}{2}P_0$ and $x_{02} = Q_0$, and the matrix becomes

$$\mathbf{M} = \begin{pmatrix} -2\,\partial X_1/\partial P_0 & \partial X_1/\partial Q_0 \\ -2\,\partial X_2/\partial P_0 & \partial X_2/\partial Q_0 \end{pmatrix}. \tag{40}$$

The determinant of $\mathbf{M}$ is easily seen to be a multiple of the Poisson bracket of X_1 and X_2:

$$\det \mathbf{M} = 2\left\{\frac{\partial X_1}{\partial Q_0}\frac{\partial X_2}{\partial P_0} - \frac{\partial X_1}{\partial P_0}\frac{\partial X_2}{\partial Q_0}\right\} = 2[X_1, X_2]_{P_0Q_0}. \tag{41}$$

In order to examine the signature of the matrix $\mathbf{M}(t'+\epsilon)\mathbf{M}^{-1}(t'-\epsilon)$ we require the inverse matrix to $\mathbf{M}$. It is

$$\mathbf{M}^{-1} = \frac{1}{2[X_1, X_2]}\begin{pmatrix} \partial X_2/\partial Q_0 & -\partial X_1/\partial Q_0 \\ 2\,\partial X_2/\partial P_0 & -2\,\partial X_1/\partial P_0 \end{pmatrix}. \tag{42}$$

That this is indeed the inverse to $\mathbf{M}$ can be proved by direct multiplication.

Focal points occur for those times t' such that $\det \mathbf{M}$ vanishes. The process (X_1, X_2) is now a function of P_0, Q_0 and t since the condition $P_i(0)=0$ has now been subsumed. We shall have (for example) a caustic at any time t' such that X_1 is a constant. Expanding X_1 to first order in a Taylor series in ϵ at times $t'\pm\epsilon$ shows that, at such a focal point (leaving out the algebra),

$$\mathbf{M}(t'+\epsilon)\,.\,\mathbf{M}^{-1}(t'-\epsilon) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

To find the contribution to $\mathbf{M}$ of such a focal point we must evaluate $(n-\sigma)/2$, where $n=2$ and the signature (the number of positive minus the number of negative eigenvalues) is $1-1=0$. The resulting contribution to $\mathbf{M}$ is unity. In general one can see that every focal point on the path contributes unity to $\mathbf{M}$. Thus, referring to equation (10), the phase changes by $-\pi/2$ at every focal point.

In § 6 we give an example of the above considerations by showing how to derive the Bohr–Sommerfeld quantisation rule for bound states.

6. Energy quantisation for bound systems

To obtain the semiclassical approximation for energy states we consider the density of states $n(E)$ given by

$$n(E) = -(1/\pi)\,\mathrm{Im}\,\mathrm{Tr}[1/(E-H)]. \tag{43}$$

The operator inside the trace may be expressed in the usual way by a Laplace integral:

$$\frac{1}{E-H} = \frac{1}{\mathrm{i}\hbar}\int_0^\infty \mathrm{d}t\, \exp\frac{\mathrm{i}}{\hbar}(E-H)t.$$

The trace of an operator is given by equation (6) with $B=1$. Thus the quantity to be approximated is

$$n(E) = \frac{1}{h}\int_{-\infty}^{\infty} \mathrm{d}t\, \exp\left(\frac{\mathrm{i}}{\hbar}Et\right)\int \frac{\mathrm{d}p\,\mathrm{d}q}{h}\,U(pqt). \tag{44}$$

Using the semiclassical approximation for the Weyl transformed propagator $U(pqt)$ gives

$$n(E) \simeq \frac{1}{h}\sum_k \int \frac{\mathrm{d}p\,\mathrm{d}q}{h}\int_{-\infty}^{\infty}\mathrm{d}t\,\frac{\exp(\mathrm{i}/\hbar)Et\,\exp(\mathrm{i}/\hbar)(S_k-(\pi\hbar/2)m_k)}{\sqrt{|\det \mathbf{M}_{ij}|}} \tag{45}$$

In equations (44) and (45) and in the following treatment we interpret $U(pq-t)$ as the complex conjugate of $U(pqt)$.

In equation (45) the matrix $\mathbf{M}$ is defined by equation (14), where S_k is the action for the kth classical path and depends upon p, q and t, and m_k is the corresponding index. Throughout, of course, the trajectories are calculated under the restriction

$P_i(0)=0$ or, what is equivalent, equations (38). If we perform the time integral in equation (45) by stationary phase then the condition is that only those times contribute (in the sense of stationary phase) such that

$$E+\partial S_k/\partial t=0. \tag{46}$$

This determines the time t as a function of E and of $(x_1, x_2)=(p, q)$, the values of X_i at time t. But S_k also satisfies the Hamilton–Jacobi equation (27), so the motion of X_i occurs on the shell $\mathscr{H}=E$.

Since equation (46) determines t as a function of p, q and E, we may define the energy-dependent action $\mathscr{S}_k$ by

$$\mathscr{S}_k(E, x_1, x_2)=Et(E, x_1, x_2)+S_k(t(E, x_1, x_2), x_1, x_2). \tag{47}$$

The integral in equation (45) on x_1 (that is p) may also be performed by stationary phase. The stationary phase condition here is

$$\partial\mathscr{S}/\partial x_1=0. \tag{48}$$

But $\partial\mathscr{S}/\partial x_1$ is the generalised momentum P_1 at the upper point (at time t). Thus only those trajectories X_i contribute (in the sense of stationary phase) such that P_1 vanishes at time t. Reference to equation (35a) shows that, interpreted for the plus and minus systems, this condition means that

$$P^+(t)=-P^-(t). \tag{49}$$

In summary, the conditions are now that equations (38a) and (38b) apply initially, whilst equation (49) applies at the later time t. Furthermore, both systems Q^+ and Q^- move on the shell $E^+=E^-=E$. Since we are assuming bound motion, these conditions mean that after time t the plus and minus systems will either have changed places on the shell in phasespace or done one or more complete circuits to return to their starting points, Thus, only times $kT/2$ contribute (with k any integer) such that T is the period for one complete circuit for the plus or minus systems. At these times $|\det \mathbf{M}|$ will equal unity, but the stationary phase integrals on t and p $(=x_1)$ do give multiplicative factors. Collecting terms, one finds

$$n(E)=\frac{2}{h}\sum_{k=-\infty}^{\infty}\int \mathrm{d}q\,\exp\left[\frac{\mathrm{i}}{\hbar}\left(\mathscr{S}_k-\frac{\pi}{2}m_k\right)\right]\Big/\left[\left(\frac{\partial^2 S_k}{\partial t^2}\right)\left(\frac{\partial^2\mathscr{S}_k}{\partial x_1^2}\right)\right]^{1/2}. \tag{50}$$

Where time $t=kT/2$ is required to satisfy (48), and the factor of 2 arises from the fact that two values of x_1 contribute, corresponding to $\pm P$ on the energy surface.

To evaluate the term inside the square root we differentiate equation (48) with respect to x_1 (holding x_2 constant) and equation (46) with respect to t, to obtain respectively

$$\frac{\partial^2\mathscr{S}_k}{\partial x_1^2}+\frac{\partial^2\mathscr{S}_k}{\partial E\,\partial x_1}\frac{\partial E}{\partial x_1}=0$$

$$\frac{\partial^2 S_k}{\partial t^2}=-\frac{\partial E}{\partial t}.$$

The pre-exponential factor in equation (50) now becomes

$$\frac{1}{(\partial^2 S_k/\partial t^2)(\partial^2\mathscr{S}_k/\partial x_1^2)}=-\left(\frac{\partial t}{\partial P_1}\right)\frac{1}{(\partial E/\partial x_1)}.$$

This is to be evaluated at times $t_k = kT/2$, and it is easy to show that

$$(\partial P_1/\partial t) = (1/2m)P^+(E, Q^+).$$

The other derivative, $\partial E/\partial x_1$, can be evaluated when we realise that, at times t_k, P_2 vanishes. This follows from equation (35*d*) and the condition that $P^+ = -P^-$ at times t_k. Condition (33*b*) implies $\mathscr{H} = E$. Thus from equation (28)

$$\partial E/\partial x_1 = x_1/m = -P^+/2m.$$

Collecting terms gives

$$n(E) \simeq \frac{2}{h}\int_a^b \mathrm{d}Q^+ \frac{2m}{P^+} \sum_{k=-\infty}^{\infty} \exp\frac{\mathrm{i}}{\hbar}\left(\mathscr{S}_k - \frac{m_k\pi}{2}\right)$$

where a and b are the turning points. In this expression we recognise the period τ as a function of energy of a bound particle, mass m, moving between turning points a and b:

$$\tau(E) = \int_a^b \frac{4m\,\mathrm{d}Q^+}{P^+} = 2\int_a^b \frac{\mathrm{d}q\, m^{1/2}}{[2(E - V(q))]^{1/2}}. \tag{51}$$

Finally we must find the phase contributions m_k of the focal points. The matrix **M** is written in equation (40) in terms of X_i. Making use of the fact that equations (38) and (35) imply that $P^-(t) = -P^+(-t)$ and $Q^-(t) = Q^+(-t)$ we may express X_i in a form emphasising the symmetry inherent in this formalism:

$$X_2 = \tfrac{1}{2}(Q^+(t) + Q^+(-t))$$
$$X_1 = -\tfrac{1}{4}(P^+(t) + P^+(-t)).$$

In general X_1 will vanish twice during each full period and (depending on the choice of origin) X_2 will be a constant *twice* during the same time. These four focal points contribute -2π phase for each complete circuit. Each half-circuit $T/2$ contributes a phase $-\pi$. Since P_1 vanishes at the upper and lower points, the first contribution to the action in equation (39) vanishes and the second two contributions are equal. We then have (with negative values of k corresponding to negative times)

$$-(\pi/2)m_k = -k\pi$$
$$\mathscr{S}_k = (k/2)\oint P^+\,\mathrm{d}Q^+ = k\oint p\,\mathrm{d}q.$$

In the last step we have related the motion of the system for mass $4m$ to the actual system, mass m, just as we did for equation (51). We thus obtain

$$n(E) \simeq (1/h)\sum_{-\infty}^{\infty} \tau(E)\cos k\left((1/\hbar)\oint p\,\mathrm{d}q - \pi\right).$$

By applying the Poisson sum formula Berry and Mount (1972) show that this expression becomes

$$n(E) \simeq \sum_{n=0}^{\infty} \delta(E - E_n)$$

where E_n is such that

$$\oint p\,\mathrm{d}q = (n + \tfrac{1}{2})h.$$

7. Discussion

Equation (22) shows that the propagator Q defined in equation (21) can be used to generate the Weyl transform of U_t. In this paper we have considered the semiclassical approximation to Q and indicated, as an example, how the corresponding semiclassical approximation for $U(pqt)$ gives rise to the usual Bohr–Sommerfeld energy quantisation rule. But Q can in principle be used to construct other interesting physical quantities. For instance, the time propagation of the Wigner function is governed by P, defined by equation (17). One may show after a little algebra that it is possible to express the propagator P in terms of $U(pqt)$ as follows:

$$P(pqt|p_0q_0 0)$$
$$= \frac{4}{h^2} \int \mathrm{d}p' \, \mathrm{d}q' \, U\left(\frac{p+p_0}{2}+p', \frac{q+q_0}{2}+q', t\right)$$
$$U^+\left(\frac{p+p_0}{2}-p', \frac{q+q_0}{2}-q', t\right) \exp\left[\frac{2\mathrm{i}}{\hbar}(p'(q-q_0)-q'(p-p_0))\right]. \qquad (52)$$

Thus a sufficiently good semiclassical approximation for the Weyl transform of U_t ought to generate an interesting approximation for P. This is being considered.

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