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An alternative approach to the semi-classical correspondence relations

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Abstract. The semi-classical correspondence relations are derived from Moshinsky's equations for the exact unitary representation of an arbitrary canonical transformation. The correspondence relations are shown to be exact in the case of a linear canonical transformation.

1. Introduction

Semi-classical mechanics, i.e. classical-limit quantum mechanics, has proved to be a source of great insight into the dynamics of a variety of physical phenomena—as, for instance, molecular scattering processes (Miller 1974, 1975). Beyond these applications semi-classical mechanics is an interesting field of theoretical physics in its own right (Berry and Mount 1972). At the very heart of this theory are the general correspondence relations as, for instance, derived by Miller (1974): the unitary representations of a canonical transformation in the semi-classical limit. The method of Miller consists of evaluating certain integral representations of quantum-mechanical matrix elements in the limit $\hbar \to 0$, i.e. by applying the method of stationary phase.

The purpose of the present paper is to show that one can arrive at the same results in a quite different way. The starting point of our proof is the work of Moshinsky *et al* (Moshinsky and Quesne 1971, Mello and Moshinsky 1975, Kramer *et al* 1978). In these papers a system of partial differential equations is derived for the unitary matrix elements representing, in quantum mechanics, a given canonical transformation of classical mechanics. Our work consists of solving these equations in the limit $\hbar \to 0$. We show that the semi-classical solution of the Moshinsky equations yields the well known correspondence relations.

In § 2 we describe briefly the derivation of Moshinsky's equations, extending his coordinate representation to momentum and mixed coordinate–momentum representations. Planck's constant $\hbar$ is retained explicitly in our formulae (and not set equal to 1). We are well aware of the numerous and profound mathematical problems which are contained in the formal arguments of § 2: unique definition of quantum operators, existence, spectra and other mathematical properties (Leaf 1969). These questions are not the subject of our paper. We essentially adopt Dirac's point of view (Dirac 1958; see also the work of Moshinsky *et al* cited above).

Section 3 deals with the semi-classical solution of Moshinsky's equations. For this purpose we introduce the amplitude and phase of the unitary matrix elements and derive a coupled system of partial differential equations for both quantities. These equations are solved in the limit $\hbar \to 0$. The phase turns out to be the generating function of the canonical transformation. To be precise, one obtains that type of generating function (Goldstein 1959) which corresponds to the chosen basis of the unitary representation. The amplitude turns out to be the related van Vleck determinant (van Vleck 1928). This is Miller's result (Miller 1974).

In § 4 we consider a linear canonical transformation. We find the semi-classical correspondence relations to be exact in this case.

2. Unitary representations of a canonical transformation

For the sake of simplicity we confine ourselves to the consideration of a one-dimensional system. The position of this system in phase-space is described by a canonically conjugate pair of variables (q, p). The corresponding quantum-mechanical operators $(\hat{q}, \hat{p})$ satisfy the commutator relation

$$[\hat{q}, \hat{p}] = \mathrm{i}\hbar. \tag{2.1}$$

Alternatively, the phase-space position of the system may also be described by a conjugate pair (Q, P) arising from (q, p) by a canonical transformation:

$$Q = g(q, p) \qquad P = h(q, p) \tag{2.2}$$

with the Poisson bracket

$$\{Q, P\}_{Q,P} = \{g, h\}_{q,p} = 1. \tag{2.3}$$

The quantum operators $(\hat{Q}, \hat{P})$ corresponding to (Q, P) are given by

$$\hat{Q} = g(\hat{q}, \hat{p}) \qquad \hat{P} = h(\hat{q}, \hat{p}) \tag{2.4}$$

satisfying

$$[\hat{Q}, \hat{P}] = \mathrm{i}\hbar. \tag{2.5}$$

According to Dirac (1958) we now assume the existence of a unitary transformation U such that

$$\hat{Q} = U\hat{q}U^{+} \qquad \hat{P} = U\hat{p}U^{+}. \tag{2.6}$$

With $U^{+} = U^{-1}$ we deduce from equations (2.4) and (2.6)

$$g(\hat{q}, \hat{p})U = U\hat{q} \tag{2.7a}$$

$$h(\hat{q}, \hat{p})U = U\hat{p}. \tag{2.7b}$$

A unitary representation of the canonical transformation (2.2) is defined as a matrix representation of the operator U in the basis of the orthonormalised eigenstates of $(\hat{q}, \hat{p})$:

$$\hat{q}|q\rangle = q|q\rangle \qquad \hat{p}|p\rangle = p|p\rangle. \tag{2.8}$$

There are four possibilities:

$$\langle q|U|Q\rangle = \langle q|Q\rangle \tag{2.9a}$$

$$\langle q|U|P\rangle = \langle q|P\rangle \tag{2.9b}$$

$$\langle p|U|Q\rangle = \langle p|Q\rangle \tag{2.9c}$$

$$\langle p|U|P\rangle = \langle p|P\rangle \tag{2.9d}$$

where

$$|Q) = U|Q\rangle \qquad |P) = U|P\rangle \tag{2.10}$$

are the eigenstates of the transformed operators $(\hat{Q}, \hat{P})$ belonging to the eigenvalues (Q, P):

$$\hat{Q}|Q) = Q|Q) \qquad \hat{P}|P) = P|P). \tag{2.11}$$

The symbols $|\rangle$ and $|)$ distinguish between eigenstates of the old and the new operators respectively.

We now establish partial differential equations for the matrix elements (2.9). For example, starting from the operator equations (2.7) one obtains for $\langle q|Q)$

$$\left[g\left(q, \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial q}\right) - Q\right]\langle q|Q) = 0 \tag{2.12a}$$

$$\left[h\left(q, \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial q}\right) + \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial Q}\right]\langle q|Q) = 0. \tag{2.12b}$$

These equations have been given by Moshinsky *et al* (Moshinsky and Quesne 1971, Mello and Moshinsky 1975, Kramer *et al* 1978). In a quite similar way we obtain such equations for the other three matrix elements:

$$\left[g\left(q, \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial q}\right) - \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial P}\right]\langle q|P) = 0 \tag{2.13a}$$

$$\left[h\left(q, \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial q}\right) - P\right]\langle q|P) = 0 \tag{2.13b}$$

$$\left[g\left(-\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial p}, p\right) - Q\right]\langle p|Q) = 0 \tag{2.14a}$$

$$\left[h\left(-\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial p}, p\right) + \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial Q}\right]\langle p|Q) = 0 \tag{2.14b}$$

$$\left[g\left(-\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial p}, p\right) - \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial P}\right]\langle p|P) = 0 \tag{2.15a}$$

$$\left[h\left(-\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial p}, p\right) - P\right]\langle p|P) = 0. \tag{2.15b}$$

As an example we sketch the derivation of equation (2.13*a*). Making use of the identities

$$\int |q'\rangle\, \mathrm{d}q' \langle q'| = \int |p'\rangle\, \mathrm{d}p' \langle p'| = 1 \tag{2.16}$$

we have from equation (2.7*a*)

$$\int \langle q|g(\hat{q}, \hat{p})|q'\rangle\, \mathrm{d}q' \langle q'|U|P\rangle = \int \langle q|U|p'\rangle\, \mathrm{d}p' \langle p'|\hat{q}|P\rangle \tag{2.17}$$

With

$$\langle q|g(\hat{q}, \hat{p})|q'\rangle = g\left(q, \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial q}\right)\delta(q - q'). \tag{2.18}$$

and

$$\langle p'|\hat{q}|P\rangle = -\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial p'}\delta(p'-P) \tag{2.19}$$

as well as the second of equations (2.10) we finally obtain equation (2.13*a*). The proof of the other equations runs in a quite analogous manner.

Moshinsky *et al* discuss exact solutions of the equations (2.12) for a variety of canonical transformations, i.e. the functions g and h. Our aim is to derive the solution of equations (2.12)–(2.15) in the limit $\hbar \to 0$ for arbitrary g and h (fulfilling condition (2.3)).

2. The semi-classical limit of a unitary representation

To calculate the matrix elements (2.9) from equations (2.12)–(2.15) we make the ansatz

$$\langle q|Q\rangle = a_1(q, Q)\exp\left(\frac{\mathrm{i}}{\hbar}b_1(q, Q)\right) \tag{3.1a}$$

$$\langle q|P\rangle = a_2(q, P)\exp\left(\frac{\mathrm{i}}{\hbar}b_2(q, P)\right) \tag{3.1b}$$

$$\langle p|Q\rangle = a_3(p, Q)\exp\left(\frac{\mathrm{i}}{\hbar}b_3(p, Q)\right) \tag{3.1c}$$

$$\langle p|P\rangle = a_4(p, P)\exp\left(\frac{\mathrm{i}}{\hbar}b_4(p, P)\right) \tag{3.1d}$$

with amplitude functions a_k and phase functions b_k to be determined. Making use of the transformation (Dirac 1958)

$$\exp\left(-\frac{\mathrm{i}}{\hbar}b(x)\right)g\left(x, \frac{\hbar}{\mathrm{i}}\frac{\mathrm{d}}{\mathrm{d}x}\right)\exp\left(\frac{\mathrm{i}}{\hbar}b(x)\right) = g\left(x, \frac{\hbar}{\mathrm{i}}\frac{\mathrm{d}}{\mathrm{d}x}+\frac{\mathrm{d}b}{\mathrm{d}x}(x)\right) \tag{3.2}$$

we obtain from (2.12)–(2.15) the equations

$$\left[g\left(q, \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial q}+\frac{\partial b_1}{\partial q}(q, Q)\right) - Q\right]a_1(q, Q) = 0 \tag{3.3a}$$

$$\left[h\left(q, \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial q}+\frac{\partial b_1}{\partial q}(q, Q)\right) + \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial Q}+\frac{\partial b_1}{\partial Q}(q, Q)\right]a_1(q, Q) = 0 \tag{3.3b}$$

$$\left[g\left(q, \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial q}+\frac{\partial b_2}{\partial q}(q, P)\right) - \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial P}-\frac{\partial b_2}{\partial P}(q, P)\right]a_2(q, P) = 0 \tag{3.4a}$$

$$\left[h\left(q, \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial q}+\frac{\partial b_2}{\partial q}(q, P)\right) - P\right]a_2(q, P) = 0 \tag{3.4b}$$

$$\left[g\left(-\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial p}-\frac{\partial b_3}{\partial p}(p, Q), p\right) - Q\right]a_3(p, Q) = 0 \tag{3.5a}$$

$$\left[h\left(-\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial p}-\frac{\partial b_3}{\partial p}(p, Q), p\right) + \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial Q}+\frac{\partial b_3}{\partial Q}(p, Q)\right]a_3(p, Q) = 0 \tag{3.5b}$$

$$\left[g\left(-\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial p}-\frac{\partial b_4}{\partial p}(p,P),p\right)-\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial P}-\frac{\partial b_4}{\partial P}(p,P)\right]a_4(p,P)=0 \tag{3.6a}$$

$$\left[h\left(-\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial p}-\frac{\partial b_4}{\partial p}(p,P),p\right)-P\right]a_4(p,P)=0. \tag{3.6b}$$

So far no special assumptions have been made. We now turn to the semi-classical limit. As a consequence, we assume that the a_k and b_k do not depend on $\hbar$. In addition, we apply the expansion (van Vleck 1928)

$$g\left(x,\frac{\hbar}{\mathrm{i}}\frac{\mathrm{d}}{\mathrm{d}x}+\frac{\mathrm{d}b}{\mathrm{d}x}(x)\right)=g\left(x,\frac{\mathrm{d}b}{\mathrm{d}x}(x)\right)+\frac{\hbar}{2\mathrm{i}}\left[\frac{\mathrm{d}}{\mathrm{d}x}g'\left(x,\frac{\mathrm{d}b}{\mathrm{d}x}(x)\right)+2g'\left(x,\frac{\mathrm{d}b}{\mathrm{d}x}(x)\right)\frac{\mathrm{d}}{\mathrm{d}x}\right]+\mathrm{O}(\hbar^2) \tag{3.7}$$

where g' means the partial derivative of the function g with respect to its second argument. Performing the expansion (3.7) in equations (3.3)–(3.6) and ordering the terms according to powers of $\hbar$ we get, as $\hbar\to 0$, two equations from each of the equations (3.3)–(3.6)—one from the terms proportional to $\hbar^0$ and the other from the terms proportional to $\hbar^1$:

$$g\left(q,\frac{\partial b_1}{\partial q}(q,Q)\right)-Q=0 \tag{3.8a}$$

$$\frac{\partial}{\partial q}\left[g'\left(q,\frac{\partial b_1}{\partial q}(q,Q)\right)a_1^2(q,Q)\right]=0 \tag{3.8b}$$

$$h\left(q,\frac{\partial b_1}{\partial q}(q,Q)\right)+\frac{\partial b_1}{\partial Q}(q,Q)=0 \tag{3.8c}$$

$$\frac{\partial}{\partial q}\left[h'\left(q,\frac{\partial b_1}{\partial q}(q,Q)\right)a_1^2(q,Q)\right]+\frac{\partial}{\partial Q}a_1^2(q,Q)=0 \tag{3.8d}$$

$$g\left(q,\frac{\partial b_2}{\partial q}(q,P)\right)-\frac{\partial b_2}{\partial P}(q,P)=0 \tag{3.9a}$$

$$\frac{\partial}{\partial q}\left[g'\left(q,\frac{\partial b_2}{\partial q}(q,P)\right)a_2^2(q,P)\right]-\frac{\partial}{\partial P}a_2^2(q,P)=0 \tag{3.9b}$$

$$h\left(q,\frac{\partial b_2}{\partial q}(q,P)\right)-P=0 \tag{3.9c}$$

$$\frac{\partial}{\partial q}\left[h'\left(q,\frac{\partial b_2}{\partial q}(q,P)\right)a_2^2(q,P)\right]=0 \tag{3.9d}$$

$$g\left(-\frac{\partial b_3}{\partial p}(p,Q),p\right)-Q=0 \tag{3.10a}$$

$$\frac{\partial}{\partial p}\left[g'\left(-\frac{\partial b_3}{\partial p}(p,Q),p\right)a_3^2(p,Q)\right]=0 \tag{3.10b}$$

$$h\left(-\frac{\partial b_3}{\partial p}(p,Q),p\right)+\frac{\partial b_3}{\partial Q}(p,Q)=0 \tag{3.10c}$$

$$\frac{\partial}{\partial p}\left[h'\left(-\frac{\partial b_3}{\partial p}(p,Q),p\right)a_3^2(p,Q)\right]-\frac{\partial}{\partial Q}a_3^2(p,Q)=0 \tag{3.10d}$$

$$g\left(-\frac{\partial b_4}{\partial p}(p,P),p\right)-\frac{\partial b_4}{\partial P}(p,P)=0 \tag{3.11a}$$

$$\frac{\partial}{\partial p}\left[g'\left(-\frac{\partial b_4}{\partial p}(p,P),p\right)a_4^2(p,P)\right]+\frac{\partial}{\partial P}a_4^2(p,P)=0 \tag{3.11b}$$

$$h\left(-\frac{\partial b_4}{\partial p}(p,P),p\right)-P=0 \tag{3.11c}$$

$$\frac{\partial}{\partial p}\left[h'\left(-\frac{\partial b_4}{\partial p}(p,P),p\right)a_4^2(p,P)\right]=0. \tag{3.11d}$$

Let us at first consider equations (3.8). From (3.8a) and (3.8c) together with the equations (2.2) we get

$$p=\frac{\partial b_1}{\partial q}(q,Q) \tag{3.12a}$$

$$P=-\frac{\partial b_1}{\partial Q}(q,Q). \tag{3.12b}$$

From these relations we conclude that the phase function $b_1(q,Q)$ is a generating function of the F_1 type (Goldstein 1959) of the canonical transformation (2.2):

$$b_1(q,Q)=F_1(q,Q). \tag{3.13}$$

Moreover, one easily verifies that equation (3.8b) as well as equation (3.8d) are solved by van Vleck's determinant (van Vleck 1928, Schiller 1962):

$$a_1(q,Q)=\left(\frac{\partial^2 F_1(q,Q)}{\partial q\,\partial Q}\right)^{1/2}. \tag{3.14}$$

Similarly, the equations (3.9)–(3.11) can be solved. We obtain

$$p=\frac{\partial b_2}{\partial q}(q,P) \tag{3.15a}$$

$$Q=\frac{\partial b_2}{\partial P}(q,P) \tag{3.15b}$$

$$q=-\frac{\partial b_3}{\partial p}(p,Q) \tag{3.16a}$$

$$P=-\frac{\partial b_3}{\partial Q}(p,Q) \tag{3.16b}$$

$$q=-\frac{\partial b_4}{\partial p}(p,P) \tag{3.17a}$$

$$Q=\frac{\partial b_4}{\partial P}(p,P). \tag{3.17b}$$

Consequently the phase functions $b_2(q,P)$, $b_3(p,Q)$, $b_4(p,P)$ are generating functions of the F_2, F_3, and F_4 type (Goldstein 1959) respectively:

$$b_2(q, P) = F_2(q, P) \tag{3.18}$$

$$b_3(p, Q) = F_3(p, Q) \tag{3.19}$$

$$b_4(p, P) = F_4(p, P). \tag{3.20}$$

Moreover, we get

$$a_2(q, P) = \left(\frac{\partial^2 F_2(q, P)}{\partial q\, \partial P}\right)^{1/2} \tag{3.21}$$

$$a_3(p, Q) = \left(\frac{\partial^2 F_3(p, Q)}{\partial p\, \partial Q}\right)^{1/2} \tag{3.22}$$

$$a_4(p, P) = \left(\frac{\partial^2 F_4(p, P)}{\partial p\, \partial P}\right)^{1/2}. \tag{3.23}$$

Formulae (3.1) together with the expressions (3.13), (3.14) and (3.18)–(3.23) define the semi-classical solution of equations (2.12)–(2.15)—up to a constant factor c. The modulus of c, i.e. the normalisation of the matrix elements (2.9), follows from the unitarity of U, which implies the conditions:

$$\int \langle q'|Q\rangle\langle q|Q\rangle^* \,\mathrm{d}Q = \delta(q' - q) \tag{3.24a}$$

$$\int \langle q'|P\rangle\langle q|P\rangle^* \,\mathrm{d}P = \delta(q' - q) \tag{3.24b}$$

$$\int \langle p'|Q\rangle\langle p|Q\rangle^* \,\mathrm{d}Q = \delta(p' - p) \tag{3.24c}$$

$$\int \langle p'|P\rangle\langle p|P\rangle^* \,\mathrm{d}P = \delta(p' - p). \tag{3.24d}$$

These equations are satisfied in the limit $\hbar \to 0$ by the above semi-classical solutions provided one chooses a normalisation factor of $|c| = (2\pi\hbar)^{-1/2}$ in each case (see the appendix). So we get the final result

$$\langle q|Q\rangle = \left|\frac{\partial^2 F_1(q, Q)}{2\pi\hbar\, \partial q\, \partial Q}\right|^{1/2} \exp\left(\frac{\mathrm{i}}{\hbar} F_1(q, Q)\right) \tag{3.25a}$$

$$\langle q|P\rangle = \left|\frac{\partial^2 F_2(q, P)}{2\pi\hbar\, \partial q\, \partial P}\right|^{1/2} \exp\left(\frac{\mathrm{i}}{\hbar} F_2(q, P)\right) \tag{3.25b}$$

$$\langle p|Q\rangle = \left|\frac{\partial^2 F_3(p, Q)}{2\pi\hbar\, \partial p\, \partial Q}\right|^{1/2} \exp\left(\frac{\mathrm{i}}{\hbar} F_3(p, Q)\right) \tag{3.25c}$$

$$\langle p|P\rangle = \left|\frac{\partial^2 F_4(p, P)}{2\pi\hbar\, \partial p\, \partial P}\right|^{1/2} \exp\left(\frac{\mathrm{i}}{\hbar} F_4(p, P)\right). \tag{3.25d}$$

These are the famous (Miller 1974) correspondence relations for the unitary representation of a canonical transformation in the semi-classical limit. A constant phase factor of modulus one remains undetermined in our derivation. In principal, one can fix the phase of the four matrix elements (3.25) in a consistent way if one makes use of the fact that the generating functions are connected by Legendre transformations (Goldstein 1959, Miller 1974).

4. Linear canonical transformations

As an example we consider a linear canonical transformation (Moshinsky and Quesne 1971)

$$Q = Aq + Bp \tag{4.1a}$$

$$P = Cq + Dp \tag{4.1b}$$

with constants A, B, C, D. The canonicity condition (2.3) demands

$$AD - BC = 1 \tag{4.2}$$

i.e. the equations (4.1) describe an orthogonal transformation of phase space. For this canonical transformation the semi-classical unitary representation of the preceding section is exact. Owing to the linearity of the functions g (and h) the linear expansion (3.7) without the term $O(\hbar^2)$ is exact, hence equations (3.8)–(3.11) are an exact consequence of equations (3.2)–(3.6). Therefore, the correspondence relations (3.25) are exact solutions of equations (2.12)–(2.15) in this case. With

$$F_1(q, Q) = -\frac{1}{2B}(Aq^2 - 2qQ + DQ^2) \qquad B \neq 0 \tag{4.3a}$$

$$F_2(q, P) = -\frac{1}{2D}(Cq^2 - 2qP - BP^2) \qquad D \neq 0 \tag{4.3b}$$

$$F_3(p, Q) = \frac{1}{2A}(Bp^2 - 2pQ - CQ^2) \qquad A \neq 0 \tag{4.3c}$$

$$F_4(p, P) = \frac{1}{2C}(Dp^2 - 2pP + AP^2) \qquad C \neq 0 \tag{4.3d}$$

formulae (3.25) yield

$$\langle q|Q\rangle = |2\pi\hbar B|^{-1/2} \exp\left(-\frac{\mathrm{i}}{2\hbar B}(Aq^2 - 2qQ + DQ^2)\right) \tag{4.4a}$$

$$\langle q|P\rangle = |2\pi\hbar D|^{-1/2} \exp\left(-\frac{\mathrm{i}}{2\hbar D}(Cq^2 - 2qP - BP^2)\right) \tag{4.4b}$$

$$\langle p|Q\rangle = |2\pi\hbar A|^{-1/2} \exp\left(\frac{\mathrm{i}}{2\hbar A}(Bp^2 - 2pQ - CQ^2)\right) \tag{4.4c}$$

$$\langle p|P\rangle = |2\pi\hbar C|^{-1/2} \exp\left(\frac{\mathrm{i}}{2\hbar C}(Dp^2 - 2pP + AP^2)\right). \tag{4.4d}$$

These matrix elements are exact unitary representations of the linear canonical transformation (4.1). This can easily be verified by insertion into equations (2.12)–(2.15) and (3.24). Concerning the phases, we refer the reader to the end of § 3. Equation (4.4a) has been derived and discussed by Moshinsky and Quesne (1971).

5. Conclusions

The correspondence relations are the central result of semi-classical mechanics. We therefore find it desirable to establish these important relations from different starting points. In this paper we have given a new approach to the correspondence relations. The significance of our method is based on the existence of equations (2.12)–(2.15) for the exact unitary representation of an arbitrary canonical transformation. The solution of these equations in the limit $\hbar \to 0$ may provide new arguments in the discussion on the range of validity of semi-classical mechanics.

Appendix

The matrix element $\langle q|Q\rangle$ is given semi-classically by

$$\langle q|Q\rangle = c\left(\frac{\partial^2 F_1(q, Q)}{\partial q\, \partial Q}\right)^{1/2} \exp\left(\frac{\mathrm{i}}{\hbar} F_1(q, Q)\right) \tag{A.1}$$

with the factor c to be determined. Insertion into the unitarity condition (3.24a) leads to

$$|c|^2 \int \left(\frac{\partial^2 F_1(q', Q)}{\partial q'\, \partial Q}\, \frac{\partial^2 F_1(q, Q)}{\partial q\, \partial Q}\right)^{1/2} \exp\left(\frac{\mathrm{i}}{\hbar}(F_1(q', Q) - F_1(q, Q)\right) \mathrm{d}Q = \delta(q' - q). \tag{A.2}$$

In the limit $\hbar \to 0$ the integrand only contributes to the integral at $q' \approx q$, so we approximate the exponent linearly:

$$F_1(q', Q) - F_1(q, Q) = \frac{\partial F_1}{\partial q}(q, Q)(q' - q) = p(q, Q)(q' - q). \tag{A.3}$$

With this approximation equation (A.2) becomes

$$|c|^2 \int \frac{\partial p}{\partial Q}(q, Q) \exp\left(\frac{\mathrm{i}}{\hbar} p(q, Q)(q' - q)\right) \mathrm{d}Q$$

$$= |c|^2 \int \exp\left(\frac{\mathrm{i}}{\hbar} p(q' - q)\right) \mathrm{d}p = \delta(q' - q); \tag{A.4}$$

hence $|c| = (2\pi\hbar)^{-1/2}$. A similar procedure leads to the same normalisation factor for the matrix elements $\langle q|P\rangle$, $\langle p|Q\rangle$ and $\langle p|P\rangle$. The phase of c cannot be deduced from the unitarity condition (3.24).

References

Berry M V and Mount K E 1972 *Rep. Prog. Phys.* **35** 315–97

Dirac P A M 1958 *The Principles of Quantum Mechanics* (London: Oxford University Press)

Goldstein H 1959 *Classical Mechanics* (New York: Addison–Wesley)

Kramer P, Moshinsky M and Seligman T H 1978 *J. Math. Phys.* **19** 683–93

Leaf B 1969 *J. Math. Phys.* **10** 1971–9

Mello P A and Moshinsky M 1975 *J. Math. Phys.* **16** 2017–28

Miller W H 1974 *Advan. Chem. Phys.* **25** 69–177

—— 1975 *Advan. Chem. Phys.* **30** 77–136

Moshinsky M and Quesne C 1971 *J. Math. Phys.* **12** 1772–80

Schiller R 1962 *Phys. Rev.* **125** 1109–15

van Vleck J H 1928 *Proc. Nat. Acad. Sci. USA* **14** 178–88