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Group theoretical techniques on phase space and the calculation of quantum mechanical propagators

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Abstract. It is shown by considering the representation of the Lie group $Sp(2N, R)\otimes N(N)$ on the phase space associated with *standard ordering* that the calculation of the quantum mechanical propagator for a general N-dimensional system with Hamiltonian quadratic in the position and momentum variables may be reduced to the calculation of the propagator for a 'free particle'.

1. Introduction

Recently there has been renewed interest in Lie algebraic methods for studying the time evolution of quantum mechanical systems with Hamiltonians which are linear in the generators of the Lie algebras. The majority of these methods are based on the use of suitable disentanglement theorems of the Baker-Campbell-Hausdorff (BCH) type (Wilcox 1967, Traux 1985) and, in particular, on the so-called Wei-Norman (WN) algebraic approach (Wei and Norman 1963). This approach involves the representation of the elements of a Lie group as an ordered product of exponentials, each containing only single generators of the group. These methods have been used to obtain the time evolution operator for a number of systems. Dattoli *et al* (1986a) have applied this technique to the harmonic oscillator with time-dependent frequency, as well as for a number of other systems with Hamiltonians that are linear combinations of the generators of certain lower-dimensional Lie algebras (Dattoli *et al* 1986a, b, c, 1987). Furthermore, Wolf and Korsch (1988) and Prants (1986) have derived the time development for two-dimensional quadratic parametric processes. Wang (1987) has used BCH formulae to calculate the spacetime propagator for a number of one-dimensional time-independent systems where the Hamiltonians were quadratic functions of the position and momentum coordinates. An interesting point of Wang's paper was that the calculation of such propagators could be reduced to that of a free-particle type of propagator by purely algebraic means. However, the method used by Wang does not generalise to higher dimensions or to time-dependent systems, and such a generalisation is by no means trivial. For higher-dimensional problems all of the above methods suffer from the difficulty that the BCH type formulae, as well as the result of the substitution of an already factorised exponential operator into the Schrödinger equation, become extremely difficult to calculate explicitly.

The main purpose of this paper is to generalise the result of Wang to higher-dimensional time-dependent quadratic systems, i.e. we show that the calculation of the propagator for such systems can be reduced to that of a free-particle type of

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propagator. The results suggest that a similar result may be achievable in the path integral calculation of propagators for these types of systems (for examples of the path integral calculations for certain of these systems see Cheng (1984, 1986)).

We note that the propagator for such systems has been obtained previously, by a method based on the eigenstates of linear time dependent invariants, in a paper by Dodonov *et al* (1975), which does not seem to be widely known. Less general results have been given by Tikochinsky (1977), Davies (1985), Kokiantonis and Castrigiano (1985) and Nassar and Berg (1986). However, the method used here is different, and furthermore the result is generated by showing that the problem of finding the propagator for a general N-dimensional quadratic system can be reduced, by algebraic means, to finding the propagator for the system with Hamiltonian

$$\hat{H}_0(t) = \hat{\boldsymbol{p}}^{\mathrm{T}} A(t) \hat{\boldsymbol{p}} \tag{1.1}$$

where $\hat{\boldsymbol{p}} = (\hat{p}_1, \hat{p}_2, \ldots, \hat{p}_N)$ and $A(t)$ is an $N \times N$ symmetric matrix and T denotes the transpose. The propagator for this system is easily calculated. First, if $N = 1$ the result is well known (Suzuki 1983):

$$\begin{aligned} K_F(A(t); x_b, t; x_a, 0) &\equiv \langle x_b | \exp(-(\mathrm{i}/\hbar) A(t) \hat{p}^2) | x_a \rangle \\ &= (4\pi \mathrm{i} \hbar A(t))^{-1/2} \exp\left(\frac{\mathrm{i}(x_b - x_a)^2}{4\hbar A(t)} \right) \end{aligned} \tag{1.2}$$

where $|x_a\rangle$ and $|x_b\rangle$ denote eigenstates of $\hat{q}$. The result in N dimensions then follows by diagonalising $A(t)$ and using (1.2):

$$\begin{aligned} &K_F(A(t); \boldsymbol{x}_b, t; \boldsymbol{x}_a, 0) \\ &\quad \equiv \langle \boldsymbol{x}_b | \exp(-(\mathrm{i}/\hbar) \hat{\boldsymbol{p}}^{\mathrm{T}} A(t) \hat{\boldsymbol{p}} | \boldsymbol{x}_a \rangle \\ &\quad = (4\pi \mathrm{i} \hbar \det A(t))^{-1/2} \exp\left(\frac{\mathrm{i}}{4\hbar} [(\boldsymbol{x}_b - \boldsymbol{x}_a)^{\mathrm{T}} A(t)^{-1} (\boldsymbol{x}_b - \boldsymbol{x}_a)] \right). \end{aligned} \tag{1.3}$$

We note another important point of the present work, namely that for systems for which the Hamiltonian is a homogeneous quadratic function of the position and momentum variables, the propagator may be written entirely in terms of $2N$ solutions of the corresponding classical system, and furthermore that this is also the case for time evolution operators of all such one-dimensional quadratic systems. This generalises a result recently obtained by Fernandez (1987) for the time development operator for the system with Hamiltonian $H = \alpha(t)\hat{p}^2 + \beta(t)\hat{q}^2$.

It is well known that the Hamiltonian of a general N-dimensional quadratic system is a linear combination of the generators of the Lie group $\mathrm{Sp}(2N, R) \otimes \mathrm{N}(N)$, i.e. the semidirect product of the semisimple simplectic group $\mathrm{Sp}(2N, R)$ and the nilpotent group $\mathrm{N}(N)$. The method of approach adopted here is to use the phase space representation associated with the so-called standard ordering (Agarwal and Wolf 1970) of the Lie group $\mathrm{Sp}(2N, R) \otimes \mathrm{N}(N)$ and its algebra. The phase space representation of the group $\mathrm{Sp}(2N, R) \otimes \mathrm{N}(N)$ and the corresponding Lie algebra are described in § 2 and algebraic phase space techniques are used to deduce the group multiplication law on the phase space.

In § 3 it is shown that one may work within the phase space in a purely algebraic manner to calculate the standard ordered form of the unitary time development operator. The standard method for finding the phase space representation of time development operators (usually in the phase space associated with *normal* or *antinormal* ordering) is to solve the phase space form of the Schrödinger equation for the time development operator (Louisell 1973, Agarawal and Wolf 1970, Howard and Roy 1987). This method has the disadvantage that it generates non-linear differential equations, which are to be compared with the (linear) classical equations of motion generated by the method described here. In § 3 we apply the results obtained to the reduction of the propagator for such systems.

2. Group theory on phase space

The Hamiltonian of a general N-dimensional quadratic system is given by

$$\hat{H}(\hat{\boldsymbol{q}}, \hat{\boldsymbol{p}}, t) = \sum_{j=1}^{N} \sum_{k=1}^{N} (a_{jk}(t)\hat{p}_j\hat{p}_k + b_{jk}(t)(\hat{q}_j\hat{p}_k + \hat{p}_k\hat{q}_j)$$
$$+ c_{jk}(t)\hat{q}_j\hat{q}_k) + \sum_{j=1}^{N} (d_j(t)\hat{p}_j + e_j(t)\hat{q}_j) + f(t) \tag{2.1}$$

where $a_{jk}(t)$, $b_{jk}(t)$ and $c_{jk}(t)$ are real $N \times N$ matrices, with $a(t)$ and $c(t)$ being symmetric, and $d_j(t)$, $e_j(t)$ and $f(t)$ are real functions. The Hamiltonian (2.1) is a linear combination of the set of operators

$$\{\hat{p}_j\hat{p}_k, \hat{q}_j\hat{p}_k + \hat{p}_k\hat{q}_j, \hat{q}_j\hat{q}_k, \hat{q}_j, \hat{p}_j, I\}$$

where j, $k = 1, \ldots, N$ and I is the identity operator. This set of operators gives a realisation of the Lie algebra $\mathrm{sp}(2N, R) \oplus \mathrm{n}(N)$. This algebra is the semidirect product of the semisimple symplectic algebra $\mathrm{sp}(2N, R)$, which is realised by the quadratic operators in the above set, and the radical $\mathrm{n}(N)$, realised by $\{q_j, p_j, I\}$, $j = 1, \ldots, N$.

We now consider the representation of the Lie algebra $\mathrm{sp}(2N, R) \oplus \mathrm{n}(N)$ in phase space and, in particular, in the phase space associated with standard ordering (Agarwal and Wolf 1970). Here we introduce the phase space representation in a purely algebraic way as follows. To obtain the phase space representation of an operator function $\hat{F}(\hat{\boldsymbol{q}}, \hat{\boldsymbol{p}})$ (all operators are assumed to have power series expansion in $\hat{p}$ and $\hat{q}$), replace the operators $\hat{q}$ and $\hat{p}$ by the corresponding c-number variables q and p, which define the phase space, and replace operator multiplication by the $*$ product which is defined to be associative and satisfy the following relations:

$$p_i * q_j = q_j p_i - \mathrm{i}\hbar\delta_{ij} \tag{2.2}$$

$$q_i * p_j = q_i p_j \tag{2.3}$$

$$f(\boldsymbol{q}, \boldsymbol{p}) * p_i = f(\boldsymbol{q}, \boldsymbol{p}) p_i \tag{2.4}$$

$$q_i * f(\boldsymbol{q}, \boldsymbol{p}) = q_i f(\boldsymbol{q}, \boldsymbol{p}) \tag{2.5}$$

$$c * f(\boldsymbol{q}, \boldsymbol{p}) = f(\boldsymbol{q}, \boldsymbol{p}) * c = c f(\boldsymbol{q}, \boldsymbol{p}) \tag{2.6}$$

where $i, j = 1, \ldots, N$, $f(\boldsymbol{q}, \boldsymbol{p})$ is any function on the phase space and c is any constant function on the phase space. Through this procedure and use of (2.2)–(2.6), an operator $\hat{F}(\hat{\boldsymbol{q}}, \hat{\boldsymbol{p}})$ may be reduced to a c-number function $F(\boldsymbol{q}, \boldsymbol{p})$, the standard ordered representative of $\hat{F}(\hat{\boldsymbol{q}}, \hat{\boldsymbol{p}})$, on the phase space. From (2.2)–(2.6) it can be readily established that

$$[q_j, p_k] \equiv q_j * p_k - p_k * q_j = \mathrm{i}\hbar\delta_{jk} \tag{2.7}$$

$$p_j^m * f(\boldsymbol{q}, \boldsymbol{p}) = \left(p_j - \mathrm{i}\hbar\frac{\partial}{\partial q_j}\right)^m f(\boldsymbol{q}, \boldsymbol{p}) \tag{2.8}$$

$$f(\boldsymbol{q}, \boldsymbol{p}) * q_j^m = \left(q_j - \mathrm{i}\hbar\frac{\partial}{\partial p_j}\right)^m f(\boldsymbol{q}, \boldsymbol{p}). \tag{2.9}$$

We then find that the phase space functions

$$\{p_j p_k,\ q_j p_k + (\mathrm{i}\hbar/2)\delta_{jk},\ q_j q_k,\ q_k,\ p_k,\ 1\}$$

form a representation of the Lie algebra $\mathrm{sp}(2N, R)\oplus \mathrm{n}(N)$ under the $*$ product.

To re-obtain an operator $\hat{F}(\hat{\boldsymbol{q}}, \hat{\boldsymbol{p}})$ from its phase space representative we simply use the rules (2.2)-(2.6) in the reverse order. That is, we replace all products between q and p by $*$ products, using (2.2)-(2.6), and then replace q_i and p_i by $\hat{q}_i$ and $\hat{p}_i$, respectively. By (2.2)-(2.6) this procedure is equivalent to writing $F(\boldsymbol{q}, \boldsymbol{p})$ in such a way that in every product all the q are to the left of all the p and then replacing q_i and p_i by $\hat{q}_i$ and $\hat{p}_i$, respectively. We denote this operator by $\mathscr{S}$:

$$\hat{F}(\hat{\boldsymbol{q}}, \hat{\boldsymbol{p}}) = \mathscr{S}\{F(\boldsymbol{q}, \boldsymbol{p})\}. \tag{2.10}$$

We now consider the representation of the group operators on the phase space. The above realisation of the Lie algebra $\mathrm{sp}(2N, R)\oplus\mathrm{n}(N)$, in terms of the operators $\hat{q}$, $\hat{p}$, $\hat{I}$ and their bilinear products, generates a unitary representation of the Lie group $\mathrm{Sp}(2N, R)\otimes \mathrm{N}(N)$, a general element of which can be written as

$$\hat{U}(A, B, C, D, E, \Phi) = \exp\left(\frac{\mathrm{i}}{\hbar}(\hat{\boldsymbol{q}}^{\mathrm{T}}A\hat{\boldsymbol{q}} + \hat{\boldsymbol{q}}^{\mathrm{T}}B\hat{\boldsymbol{p}} + \hat{\boldsymbol{p}}^{\mathrm{T}}B^{\mathrm{T}}\hat{\boldsymbol{q}} + \hat{\boldsymbol{p}}^{\mathrm{T}}C\hat{\boldsymbol{p}} + D^{\mathrm{T}}\hat{\boldsymbol{q}} + E^{\mathrm{T}}\hat{\boldsymbol{p}} + \Phi\hat{I})\right).$$

Using the parameter differentiation method of Wilcox (1967) it can be shown that $\hat{U}$ can be written in the partially factorised form

$$\hat{U}(\alpha, \tau, \gamma, \delta, \varepsilon, \phi) \equiv \exp\left(\frac{\mathrm{i}}{\hbar}\phi\hat{I}\right)\exp\left(\frac{\mathrm{i}}{\hbar}(\hat{\boldsymbol{q}}^{\mathrm{T}}\alpha\hat{\boldsymbol{q}} + \delta^{\mathrm{T}}\hat{\boldsymbol{q}})\right)$$
$$\times\exp\left(\frac{\mathrm{i}}{\hbar}(\hat{\boldsymbol{q}}^{\mathrm{T}}\tau\hat{\boldsymbol{p}} + \hat{\boldsymbol{p}} + \hat{\boldsymbol{p}}^{\mathrm{T}}\tau^{\mathrm{T}}\hat{\boldsymbol{q}})\right)\exp\left(\frac{\mathrm{i}}{\hbar}(\hat{\boldsymbol{p}}^{\mathrm{T}}\gamma\hat{\boldsymbol{p}} + \varepsilon^{\mathrm{T}}\hat{\boldsymbol{p}})\right). \tag{2.11}$$

The relationship between the group parameters $A, \ldots, \Phi$ and $\alpha, \ldots, \phi$ does not concern us here. The representation of this general element in the phase space is then obtained by the use of the prescription described above as well as the result (A5) of the appendix. The result is

$$U(\alpha, \beta, \gamma, \delta, \varepsilon, \phi) = \exp(\mathrm{i}\phi/\hbar)D(\delta, \varepsilon)S(\alpha, \beta, \gamma) \tag{2.12}$$

where

$$D(\delta, \varepsilon) = \exp\left(\frac{\mathrm{i}}{\hbar}(\varepsilon^{\mathrm{T}}\boldsymbol{p} - \delta^{\mathrm{T}}\boldsymbol{q})\right) \tag{2.13}$$

$$S(\alpha, \beta, \gamma) = (\det\beta)^{1/2}\exp\left(\frac{\mathrm{i}}{\hbar}(\boldsymbol{q}^{\mathrm{T}}\alpha\boldsymbol{q} + \boldsymbol{q}^{\mathrm{T}}(\beta^{\mathrm{T}} - I)\boldsymbol{p} + \boldsymbol{p}^{\mathrm{T}}\gamma\boldsymbol{p})\right) \tag{2.14}$$

and $\beta^T = \exp(2\tau)$.

For completeness we now calculate the group multiplication law with the use of phase space methods. The functions $S(\alpha, \beta, \gamma)$ form the phase space representation of the group $\mathrm{Sp}(2N, R)$, so we first calculate the group multiplication law for this group. We first calculate the effect of the phase space operators S on the functions $\boldsymbol{p}$ and $\boldsymbol{q}$. We have, using (2.8) and (2.9),

$$S^{\dagger}(\alpha, \beta, \gamma) * S(\alpha, \beta, \gamma) = S^{\dagger} * S * q_j + \mathrm{i}\hbar S^{\dagger} * \frac{\partial S}{\partial p_j} \tag{2.15}$$

where $S^{\dagger}$ denotes the phase space representative of the operator $\hat{S}^{\dagger}$ with $\hat{S} = \mathscr{S}\{S\}$. Along with (2.14), (2.15) then gives

$$S^{\dagger} * \boldsymbol{q} * S = \beta^{-1}\boldsymbol{q} - 2\beta^{-1}\gamma \boldsymbol{p}. \tag{2.16}$$

In a similar way using (2.8), (2.14) and (2.16) we obtain

$$S^{\dagger} * \boldsymbol{p} * S = (\beta^{\mathrm{T}} - 4\alpha\beta^{-1}\gamma)\boldsymbol{p} + 2\alpha\beta^{-1}\boldsymbol{q}. \tag{2.17}$$

Applying both sides of the relation

$$S(\alpha_3, \beta_3, \gamma_3) = S(\alpha_1, \beta_1, \gamma_1) * S(\alpha_2, \beta_2, \gamma_2) \tag{2.18}$$

to p_j and q_j comparing we find that

$$\beta_3 = \beta_2(I - 4\gamma_1\alpha_2)^{-1}\beta_1 \tag{2.19a}$$

$$\alpha_3 = \alpha_1 + \beta_1^{\mathrm{T}}\alpha_2(I - 4\gamma_1\alpha_2)^{-1}\beta_1 \tag{2.19b}$$

$$\gamma_3 = \gamma_2 + \beta_2(I - 4\gamma_1\alpha_2)^{-1}\gamma_1\beta_2^{\mathrm{T}}. \tag{2.19c}$$

Equation (2.18), together with (2.19), constitute the group multiplication law for the group $\mathrm{Sp}(2N, R)$ on the phase space. To obtain the full group multiplication law we use the following simply derived consequences of (2.8) and (2.9):

$$\exp\left(-\frac{\mathrm{i}}{\hbar}\varepsilon^{\mathrm{T}}\boldsymbol{p}\right) * q_j * \exp\left(\frac{\mathrm{i}}{\hbar}\varepsilon^{\mathrm{T}}\boldsymbol{p}\right) = q_j - \varepsilon_j \tag{2.20a}$$

and

$$\exp\left(\frac{\mathrm{i}}{\hbar}\delta^{\mathrm{T}}\boldsymbol{q}\right) * p_j * \exp\left(-\frac{\mathrm{i}}{\hbar}\delta^{\mathrm{T}}\boldsymbol{q}\right) = p_j - \delta_j. \tag{2.20b}$$

The full group multiplication law now follows by collapsing the $*$ product in

$$U(\alpha_3, \beta_3, \gamma_3, \delta_3, \varepsilon_3, \phi_3) = U(\alpha_1, \beta_1, \gamma_1, \delta_1, \varepsilon_1, \phi_1) * U(\alpha_2, \beta_2, \gamma_2, \delta_2, \varepsilon_2, \phi_2) \tag{2.21}$$

using (2.18)-(2.20). The result is

$$\phi_3 = \phi_1 + \phi_2 - \delta_2^{\mathrm{T}}\varepsilon_1 + \delta_2^{\mathrm{T}}\gamma_1\delta_2 + \varepsilon_1^{\mathrm{T}}\alpha_2\varepsilon_1 \tag{2.22a}$$

$$\delta_3 = \delta_1 + \delta_2 - 2\varepsilon_2^{\mathrm{T}}\alpha_2 + \delta_2^{\mathrm{T}}(\beta_2 - I) \tag{2.22b}$$

$$\varepsilon_3 = \varepsilon_1 + \varepsilon_2 - 2\delta_2^{\mathrm{T}}\gamma_1 + \varepsilon_1(\beta_2^{\mathrm{T}} - I) \tag{2.22c}$$

along with (2.19).

3. Algebraic calculation of the phase space representation of $\hat{U}(t)$

We first calculate the phase space representation of the time evolution operator. The usual method for calculating the phase space representatives (usually in the phase space associated with normal or antinormal ordering) of time evolution operators is to solve the phase space form of the Schrödinger equation for the operator $U(t)$, i.e.

$$\mathrm{i}\hbar\frac{\partial \hat{U}}{\partial t}=\hat{H}(t)\hat{U} \qquad \hat{U}(0)=\hat{I}. \tag{3.1}$$

In the case of standard ordering, (3.1) takes the form

$$\mathrm{i}\hbar\frac{\partial U}{\partial t}=H(t)*U \qquad U(0)=1 \tag{3.2}$$

where $*$ was defined in the previous section. Equation (3.2) is then solved by assuming U has a particular form (Louisell 1973). The main difficulty with this approach is that it generates non-linear differential equations. Here we use an algebraic method on the phase space similar to the one used in the previous section to calculate the phase space form of the operator $\hat{U}(t)$.

In the Heisenberg picture the position and momentum operatos $\hat{q}_j$ and $\hat{p}_j$ must satisfy the equations of motion:

$$\mathrm{i}\hbar\dot{\hat{q}}_j=[\hat{q}_j,\hat{H}(t)] \tag{3.3}$$

$$\mathrm{i}\hbar\dot{\hat{p}}_j=[\hat{p}_j,\hat{H}(t)]. \tag{3.4}$$

Using (2.2)-(2.6) these equations become

$$\dot{q}_j=\partial H(t)/\partial p_j \tag{3.5}$$

$$\dot{p}_j=-\partial H(t)/\partial q_j \tag{3.6}$$

in the phase space. We note that (3.5) and (3.6) are Hamilton's equations of motion with a 'classical' Hamiltonian $H(t)$. With $\hat{H}(t)$ given by (2.1), with $d_j=e_j=f=0$, $j=1,\ldots,N$ (non-zero values of these functions will be considered later), we find

$$H(t)=\sum_{j=1}^{N}\sum_{k=1}^{N}(a_{jk}(t)p_jp_k+2b_{jk}(t)p_kq_j+c_{jk}(t)q_jq_k)-\mathrm{i}\hbar\sum_{j=1}^{N}b_{jj}(t). \tag{3.7}$$

This is the classical Hamiltonian for the system (2.1). The complex term does not affect the equations of motion and so is of no consequence. With (3.7), (3.5) and (3.6) then become

$$\dot{q}_j=2\sum_{k=1}^{N}(a_{jk}(t)p_k+b_{kj}(t)q_k) \tag{3.8a}$$

and

$$\dot{p}_j=-2\sum_{k=1}^{N}(b_{jk}(t)p_k+c_{jk}(t)q_k). \tag{3.8b}$$

Given the initial conditions $q_j(0)$ and $p_j(0)$, the solution of (3.8) is well known to exist and be unique. We write this solution in the form

$$q_j(t)=\sum_{k=1}^{N}\{[Q_j^1]_kp_k(0)-[Q_j^2]_kq_k(0)\} \tag{3.9}$$

$$p_j(t)=\sum_{k=1}^{N}\{[P_j^1]_kp_k(0)-[P_j^2]_kq_k(0)\} \tag{3.10}$$

where Q_j^1, P_j^1 and Q_j^2, P_j^2, $j=1,\ldots,N$, are the $2N$ unique classical solutions satisfying the initial conditions $[Q_j^1]_k=[P_j^2]_k=0$ and $-[Q_j^2]_k=[P_j^1]_k=\delta_{jk}$. For convenience we define the matrices

$$[\Lambda_l]_{jk}=[Q_j^l]_k \tag{3.11}$$

$$[M_l]_{jk}=[P_j^l]_k \tag{3.12}$$

where $l=1,2$ and $j,k=1,\ldots,N$. It may be verified that

$$M_2(t)\Lambda_1^{\mathrm{T}}(t)-\Lambda_2(t)M_1^{\mathrm{T}}(t)=I_{N\times N} \tag{3.13}$$

for all time, the right-hand side denoting the $N\times N$ identity matrix.

We now use (3.7) and (3.8) to calculate the phase space representative of $\hat{U}(t)$ for this system algebraically. Suppose that $U(t)$ is of the form (2.14) and $U^\dagger(t)$ is the phase space representative of $\hat{U}^\dagger(t)$ so that

$$U^\dagger(t)*U(t)=U(t)*U^\dagger(t)=1. \tag{3.14}$$

In what follows we do not need the explicit form of $U^\dagger(t)$; we need only (3.14).

To find $U(t)$ we now just calculate $U^\dagger(t)*q_j*U(t)$ and $U^\dagger(t)*p_j*U(t)$ and compare with (3.9) and (3.10). Using (2.8) and (2.14) we find

$$\begin{aligned}q_j(t)&=U^\dagger(t)*q_j*U(t)=U^\dagger(t)*U(t)*q_j+\mathrm{i}\hbar U^\dagger(t)*\frac{\partial U}{\partial p_j}\\&=q_j-\sum_{k=1}^{N}(2\gamma_{jk}p_k+(\beta^{\mathrm{T}}-I)_{kj}U^\dagger(t)*q_k*U(t))\end{aligned} \tag{3.15}$$

or in matrix notation we obtain

$$\boldsymbol{q}(t)=\beta^{-1}\boldsymbol{q}-2\beta^{-1}\gamma\boldsymbol{p}. \tag{3.16}$$

In a similar way we obtain, using (3.16),

$$\begin{aligned}\boldsymbol{p}(t)&=\beta^{\mathrm{T}}\boldsymbol{p}+2\alpha\boldsymbol{q}(t)\\&=(\beta^{\mathrm{T}}-4\alpha\beta^{-1}\gamma)\boldsymbol{p}+2\alpha\beta^{-1}\boldsymbol{q}.\end{aligned} \tag{3.17}$$

Comparing (3.16) and (3.17) with (3.9) and (3.10) we find

$$\beta=-\Lambda_2^{-1}\qquad\alpha=\tfrac{1}{2}M_2\Lambda_2^{-1}\qquad\gamma=\tfrac{1}{2}\Lambda_2^{-1}\Lambda_1. \tag{3.18}$$

By considering the differential equations satisfied by Λ and M and the corresponding initial conditions it may be checked that α and γ defined by (3.18) are indeed symmetric. Furthermore, by using (3.13) and the symmetry of α and γ we find $\beta^{\mathrm{T}}-4\alpha\beta^{-1}\gamma=M_1$. Hence the phase space representative of the time development operator $\hat{U}(t)$ is

$$U(t)=(-1)^{N/2}(\det\Lambda_2)^{-1/2}\exp\left(\frac{\mathrm{i}}{\hbar}\{\tfrac{1}{2}\boldsymbol{p}^{\mathrm{T}}\Lambda_2^{-1}\Lambda_1\boldsymbol{p}-\boldsymbol{q}^{\mathrm{T}}[I+(\Lambda_2^{\mathrm{T}})^{-1}]\boldsymbol{p}+\tfrac{1}{2}\boldsymbol{q}M_2\Lambda_2^{-1}\boldsymbol{q}\}\right) \tag{3.19}$$

and so using (2.13) and (2.15) we have

$$\begin{aligned}\hat{U}(t)=(-1)^{N/2}&(\det\Lambda_2)^{-1/2}\exp\left(\frac{\mathrm{i}}{2\hbar}\boldsymbol{q}M_2\Lambda_2^{-1}\boldsymbol{q}\right)\\&\times\mathcal{S}\left[\exp\left(-\frac{\mathrm{i}}{\hbar}\boldsymbol{q}^{\mathrm{T}}[I+(\Lambda_2^{\mathrm{T}})^{-1}]\boldsymbol{p}\right)\right]\exp\left(\frac{\mathrm{i}}{2\hbar}\boldsymbol{p}^{\mathrm{T}}\Lambda_2^{-1}\Lambda_1\boldsymbol{p}\right).\end{aligned} \tag{3.20}$$

We look at some interesting special cases of (3.20). For the one-dimensional case $\Lambda_{1,2} = Q_{1,2}$ and $M_{1,2} = P_{1,2}$ where $Q_{1,2}$ and $P_{1,2}$ are a pair of classical solutions for the system, i.e.

$$\dot{Q}_{1,2} = 2\{a(t)P_{1,2} + b(t)Q_{1,2}\}$$
$$\dot{P}_{1,2} = -2\{b(t)P_{1,2} + c(t)Q_{1,2}\}$$

satisfying the initial conditions $Q_1(0) = P_2(0) = 0$ and $-Q_2(0) = P_1(0) = 1$. In this case we may invert the transformation (2.10) to obtain $\hat{U}(t)$ as a product of exponentials of the original operator algebra:

$$\hat{U}(t) = \exp\left(\frac{\mathrm{i}}{2\hbar}\frac{P_2}{Q_2}\hat{q}^2\right)\exp\left(-\frac{\mathrm{i}}{2\hbar}\log(-Q_2)(\hat{q}\hat{p}+\hat{p}\hat{q})\right)\exp\left(\frac{\mathrm{i}}{2\hbar}\frac{Q_1}{Q_2}\hat{p}^2\right). \tag{3.21}$$

This is a generalisation of a result given recently by Fernandez (1987) who showed how to write the time evolution operator for the system with Hamiltonian $H(t) = a(t)p^2 + c(t)q^2$ in terms of two classical solutions.

If the Hamiltonian is independent of time then, in general, $\hat{U}(t)$ is given by

$$\hat{U}(t) = \exp\left(\frac{\mathrm{i}}{2\hbar}\hat{\boldsymbol{q}}^{\mathrm{T}}M_2\Lambda_2^{-1}\hat{\boldsymbol{q}}\right)\exp\left(-\frac{\mathrm{i}}{2\hbar}(\hat{\boldsymbol{q}}^{\mathrm{T}}\Lambda_2^{\mathrm{T}}\dot{\Lambda}_2^{\mathrm{T}}\hat{\boldsymbol{p}}+\hat{\boldsymbol{p}}^{\mathrm{T}}\dot{\Lambda}_2\Lambda_2^{-1}\hat{\boldsymbol{q}})\right)$$
$$\times\exp\left(\frac{\mathrm{i}}{2\hbar}\hat{\boldsymbol{p}}^{\mathrm{T}}\Lambda_2^{-1}\Lambda_1\hat{\boldsymbol{p}}\right) \tag{3.22}$$

in terms of $2N$ classical solutions (apart from a time derivative in the second factor).

It is interesting to note here that the above results imply that the Schrödinger equation for systems described by Hamiltonians of the form (2.1) with $d_j = e_j = f = 0$, i.e.

$$\mathrm{i}\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle \tag{3.23}$$

may be transformed to the free-particle form:

$$\mathrm{i}\hbar\frac{\partial}{\partial t}|\phi(t)\rangle = \tfrac{1}{2}\hat{\boldsymbol{p}}^{\mathrm{T}}\frac{\mathrm{d}}{\mathrm{d}t}(\Lambda_2^{-1}\Lambda_1)\hat{\boldsymbol{p}}|\phi(t)\rangle \tag{3.24}$$

by the transformation

$$|\psi(t)\rangle = (-1)^{N/2}(\det\Lambda_2)^{-1/2}\exp\left(\frac{\mathrm{i}}{2\hbar}\boldsymbol{q}M_2\Lambda_2^{-1}\boldsymbol{q}\right)$$
$$\times\mathcal{S}\left[\exp\left(-\frac{\mathrm{i}}{\hbar}\boldsymbol{q}^{\mathrm{T}}[I+(\Lambda_2^{\mathrm{T}})^{-1}]\boldsymbol{p}\right)\right]|\phi(t)\rangle. \tag{3.25}$$

For example, the simple harmonic oscillator described by the Hamiltonian

$$\hat{H} = \tfrac{1}{2}\hat{p}^2 + \tfrac{1}{2}m\omega^2 q^2$$

can be transformed into the system described by the Hamiltonian

$$\hat{H} = \frac{1}{2m}\sec^2(\omega t)\hat{p}^2$$

via the transformation

$$|\psi(t)\rangle = \exp\left(\frac{\mathrm{i}m\omega}{2\hbar}\tan\omega t\hat{q}^2\right)\exp\left(-\frac{\mathrm{i}}{2\hbar}\log(\cos\omega t)(\hat{q}\hat{p}+\hat{p}\hat{q})\right)|\phi(t)\rangle.$$

4. Reduction of the propagator to free-particle form

Now consider the reduction of the propagator for the system with Hamiltonian (3.7) to that of a free-particle system. The propagator is obtained from

$$K(\boldsymbol{x}_b, t; \boldsymbol{x}_a, 0) \equiv \langle \boldsymbol{x}_b | \hat{U}(\hat{\boldsymbol{q}}, \hat{\boldsymbol{p}}, t) | \boldsymbol{x}_a \rangle \tag{4.1}$$

where $\hat{U}(\hat{\boldsymbol{q}}, \hat{\boldsymbol{p}}, t)$ is given by (3.20). Since (3.20) is ordered so that all the $\hat{q}_j$ are to the left of all the $\hat{p}_j$ we have

$$\begin{aligned} K(\boldsymbol{x}_b, t; \boldsymbol{x}_a, 0) &= \langle \boldsymbol{x}_b | \hat{U}(\boldsymbol{x}_b, \hat{\boldsymbol{p}}, t) | \boldsymbol{x}_a \rangle \\ &= (-1)^{N/2} (\det \Lambda_2)^{-1/2} \exp\left(\frac{\mathrm{i}}{2\hbar} \boldsymbol{x}_b^{\mathrm{T}} M_2 \Lambda_2^{-1} \boldsymbol{x}_b\right) \\ &\quad \langle \boldsymbol{x}_b | \exp\left(-\frac{\mathrm{i}}{\hbar} \boldsymbol{x}_b^{\mathrm{T}} [I + (\Lambda_2^{\mathrm{T}})^{-1}] \boldsymbol{p}\right) \exp\left(\frac{\mathrm{i}}{2\hbar} \boldsymbol{p}^{\mathrm{T}} \Lambda_2^{-1} \Lambda_1 \boldsymbol{p}\right) | \boldsymbol{x}_a \rangle . \end{aligned} \tag{4.2}$$

Using the identity

$$\langle \boldsymbol{x}_b | \exp\left(-\frac{\mathrm{i}}{\hbar} \lambda^{\mathrm{T}} \boldsymbol{p}\right) = | \boldsymbol{x}_b - \lambda \rangle \tag{4.3}$$

we finally obtain

$$\begin{aligned} K(\boldsymbol{x}_b, t; \boldsymbol{x}_a, 0) &= (-1)^{N/2} (\det \Lambda_2)^{-1/2} \exp\left(\frac{\mathrm{i}}{2\hbar} \boldsymbol{x}_b^{\mathrm{T}} M_2 \Lambda_2^{-1} \boldsymbol{x}_b\right) \\ &\quad \times K_F(-\tfrac{1}{2}\Lambda_2^{-1}\Lambda_1; \Lambda_2^{-1}\boldsymbol{x}_b, t; \boldsymbol{x}_a, 0). \end{aligned} \tag{4.4}$$

The explicit form of the propagator can be written down using the expression for K_F in § 1. We notice from the explicit form of the propagator that no difficulty arises when $\det \Lambda_2 = 0$, provided that Λ_2 is not identically zero. However, in this case the standard ordered form of the operator $\hat{U}(\hat{\boldsymbol{q}}, \hat{\boldsymbol{p}}, t)$ fails to exist, and so the propagator should be checked at these points by direct substitution in the Schrödinger equation for the propagator.

We finally consider the case in which linear terms also appear in the Hamiltonian, that is, $\boldsymbol{d}(t)$, $\boldsymbol{e}(t)$ and $f(t)$ are non-zero. In this case the 'classical' equations of motion on the phase space are

$$\dot{\boldsymbol{q}}(t) = 2a(t)\boldsymbol{p} + 2b(t)\boldsymbol{q} + \boldsymbol{e}(t) \tag{4.5}$$

and

$$\dot{\boldsymbol{p}}(t) = -2b(t)\boldsymbol{p} - 2c(t)\boldsymbol{q} - \boldsymbol{d}(t). \tag{4.6}$$

The solution to these equations is given by

$$\begin{aligned} \boldsymbol{q}(t) &= \Lambda_1 \boldsymbol{p}(0) - \Lambda_2 \boldsymbol{q}(0) - \Lambda_2 \int_0^t (M_1^{\mathrm{T}} \boldsymbol{e}(t) - \Lambda_1^{\mathrm{T}} \boldsymbol{d}(t))\, \mathrm{d}t + \Lambda_1 \\ &\quad \times \int_0^t (M_2^{\mathrm{T}} \boldsymbol{e}(t) - \Lambda_2^{\mathrm{T}} \boldsymbol{d}(t))\, \mathrm{d}t \end{aligned} \tag{4.7}$$

and

$$p(t)=M_1p(0)-M_2q(0)-M_2\int_0^t(M_1^{\mathrm{T}}e(t)-\Lambda_1^{\mathrm{T}}d(t))\,\mathrm{d}t+M_1$$
$$\times\int_0^t(M_2^{\mathrm{T}}e(t)-\Lambda_2^{\mathrm{T}}d(t))\,\mathrm{d}t \tag{4.8}$$

where $\Lambda_{1,2}$ and $M_{1,2}$ are given by (3.11) and (3.12) with Q_j^1, P_j^1 and Q_j^2, P_j^2, $j=1,\ldots,N$, being $2N$ solutions for the classical system with Hamiltonian (3.7) satisfying the initial conditions $[Q_j^1]_k=[P_j^2]_k=0$ and $-[Q_j^2]_k=[P_j^1]_k=\delta_{jk}$. Taking the phase space representative of the unitary time development operator to have the form (2.12) we find in a similar way to (2.16) and (2.17) that

$$U^{\dagger}(t)*q*U(t)=\beta^{-1}q-2\beta^{-1}\gamma p-\beta^{-1}\varepsilon \tag{4.9}$$

and

$$U^{\dagger}(t)*p*U(t)=(\beta^{\mathrm{T}}-4\alpha\beta^{-1}\gamma)p+2\alpha\beta^{-1}q-2\alpha\beta^{-1}\varepsilon-\delta. \tag{4.10}$$

Comparing (4.7) and (4.8) with (4.9) and (4.10) we find that α, β and γ are given by (3.18) and ε and δ are given by

$$\varepsilon=-\int_0^t(M_1^{\mathrm{T}}e(t)-\Lambda_1^{\mathrm{T}}d(t))\,\mathrm{d}t+\Lambda_2\Lambda_1\int_0^t(M_2^{\mathrm{T}}e(t)-\Lambda_2^{\mathrm{T}}d(t))\,\mathrm{d}t \tag{4.11}$$

and

$$\delta=2M_2\int_0^t(M_1^{\mathrm{T}}e(t)-\Lambda_1^{\mathrm{T}}d(t))\,\mathrm{d}t-(M_2\Lambda_2\Lambda_1+M_1)\int_0^t(M_2^{\mathrm{T}}e(t)-\Lambda_2^{\mathrm{T}}d(t))\,\mathrm{d}t. \tag{4.12}$$

Finally we must calculate the phase term ϕ. In order to do this we substitute $U(t)$ into the phase space form of the Schrödinger equation for the time development operator:

$$\mathrm{i}\hbar\frac{\partial U(t)}{\partial t}=H(t)*U(t) \tag{4.13}$$

with $U(0)=1$. Using

$$U*p*U^{\dagger}=\beta^{-1\mathrm{T}}(p+2\alpha q+\delta) \tag{4.14}$$

which can be obtained in a similar way to (3.16), we obtain

$$\phi=\int_0^t(\delta^{\mathrm{T}}a(t)\delta-e(t)\delta+f(t))\,\mathrm{d}t \tag{4.15}$$

where δ is given by (4.12). The propagator may then be reduced to the free-particle type as above, giving

$$K(x_b,t;x_a,0)$$
$$=(-1)^{N/2}(\det\Lambda_2)^{-1/2}\exp\left(\frac{\mathrm{i}}{\hbar}\phi\right)\exp\left(\frac{\mathrm{i}}{2\hbar}(x_bM_2\Lambda_2^{-1}x_b-2\delta^{\mathrm{T}})\right)$$
$$\times K_F(-\tfrac{1}{2}\Lambda_2^{-1}\Lambda_1;-\Lambda_2^{-1}x_b-\varepsilon,t;x_a,0) \tag{4.16}$$

where ε, δ and ϕ are given by (4.11), (4.12) and (4.15).

5. Conclusion

By considering the representation of the group $\mathrm{Sp}(2N, R)\otimes\mathrm{N}(N)$ on the quantum mechanical phase space associated with standard ordering, we have shown that the calculation of the propagator for a system driven by a general time-dependent Hamiltonian quadratic in the position and momentum operators could be reduced to the calculation of the propagator for the 'free-particle' system with Hamiltonian (1.1). Furthermore, the calculation was carried out in a purely algebraic manner. Another important result of this paper is that the propagator for a purely quadratic time-dependent system can be written entirely in terms of $2N$ solutions to the corresponding classical system.

In this paper we have also shown that the use of group theory on phase space can simplify phase space calculations. For example, the usual calculation of the phase representative of time development operators U, which involves substitution of an assumed form for the representative in the phase space form of the Schrödinger equation for $\hat{U}$, gives a set of non-linear differential equations, whereas the algebraic method used in this paper involves only the solution of a set of linear equations—the classical equations of motion.

Appendix

In this appendix we calculate the phase space representative of the operator

$$\hat{F}(\lambda)=\exp\left(\frac{2\lambda\mathrm{i}}{\hbar}\hat{\boldsymbol{q}}\tau\hat{\boldsymbol{p}}\right) \tag{A1}$$

by use of the parameter differentiation method of Wilcox (1967) in conjunction with phase space methods. The operator $\hat{F}(\lambda)$ satisfies the differential equation

$$\frac{\partial\hat{F}(\lambda)}{\partial\lambda}=\frac{2\mathrm{i}}{\hbar}\hat{\boldsymbol{q}}^{\mathrm{T}}\tau\hat{\boldsymbol{p}}\hat{F}(\lambda) \tag{A2}$$

with the initial condition $\hat{F}(0)=I$. Using (2.8) and (2.9), (A2) implies that the phase space representative of $\hat{F}(\lambda)$ satisfies

$$\frac{\partial F(\lambda)}{\partial\lambda}-2\boldsymbol{q}^{\mathrm{T}}\tau\nabla_{q}F(\lambda)=\frac{2\mathrm{i}}{\hbar}\boldsymbol{q}^{\mathrm{T}}\tau\boldsymbol{p}F(\lambda) \tag{A3}$$

with $F(0)=1$. Solving (A3) we find

$$F(\lambda)=\exp\left(\frac{\mathrm{i}}{\hbar}[\boldsymbol{q}^{\mathrm{T}}(\exp(2\lambda\tau)-I)\boldsymbol{p}]\right). \tag{A4}$$

Setting $\lambda=1$ we obtain the result used in § 2:

$$\exp 2\frac{\mathrm{i}}{\hbar}(\hat{\boldsymbol{q}}^{\mathrm{T}}\tau\hat{\boldsymbol{p}})=\mathscr{S}\left[\exp\left(\frac{\mathrm{i}}{\hbar}[\boldsymbol{q}^{\mathrm{T}}(\beta^{\mathrm{T}}-I)\boldsymbol{p}]\right)\right] \tag{A5}$$

where $\beta^{\mathrm{T}}=\exp(2\tau)$.

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