Exact eigenvalues of the Hamiltonian P^2+A mod X mod ^{nu}

1979 J. Phys. A: Math. Gen. 12 451

(http://iopscience.iop.org/0305-4470/12/4/006)

J. Phys. A: Math. Gen., Vol. 12, No. 4, 1979. Printed in Great Britain

Exact eigenvalues of the Hamiltonian $P^2 + A|X|^{\nu}$†

H Turschner

Theoretische Festkörperphysik, Technische Hochschule Darmstadt, D-6100 Darmstadt, Federal Republic of Germany

Received 14 August 1978, in final form 16 October 1978

Abstract. The correspondence between operators on a Hilbert space and phase-space functions based upon symmetric ordering, introduced by Cahill and Glauber (Weyl correspondence) is used in the present paper to define (non-linear) unitary transformations for quantum systems with the help of canonical transformations, which are bijective, i.e. one-to-one onto. These unitary transformations can be used to determine exactly the energy eigenvalues of a large class of one-dimensional quantum systems. As an example we have calculated the exact eigenvalues of the Hamiltonian $H(X, P) = \frac{1}{2m}(P^2 + a^{\frac{1}{2}(\nu+2)}|X|^{\nu})$, $a, \nu > 0$.

1. Introduction

In classical mechanics one can make a transformation from the canonical coordinate and momentum x, p to a new set of variables $\bar{x}, \bar{p}$, satisfying the same Poisson-bracket relations as the x's and p's, and can express all dynamical variables in terms of the $\bar{x}$'s and $\bar{p}$'s. These so-called canonical transformations are a powerful tool for studying the dynamic of any classical system (e.g. Goldstein 1963). In quantum mechanics the dynamic of a system is completely known if the eigenvalue problem of its Hamiltonian has been solved. This diagonalisation can be achieved by a unitary transformation from the canonical coordinate and momentum operators X and P to a new set of operators $\bar{X}$, $\bar{P}$, satisfying the same commutator relations as the X's and P's. Now there is some physical feeling that for a quantum system that has a classical analogue, unitary transformations in the quantum theory are the analogue of canonical transformations in the classical theory (see e.g. Dirac 1958). While the situation with the representation of groups of *linear* canonical transformations by groups of *linear* unitary transformation in quantum mechanics (rotation or permutation of coordinates) was clarified, it remained more obscure in the more general case, in which the new coordinates and momenta are (non-linear) functions of both the old. A detailed discussion of the problems involved in the nonlinear case may be found in a paper of Kramer *et al* (1978). Here we only want to stress the following: The operators X, P and $\bar{X}$, $\bar{P}$ may have different spectra, as happens for example in the trivial non-linear point transformation $\bar{x} = x^2$, showing that there exist canonical transformations, which cannot have a *unitary* representation in quantum theory, because unitary transformations preserve the spectra of the operators.

We therefore look for a certain class of canonical transformations which we can use to define unitary transformations. This class consists of bijective canonical transformations, i.e. mappings of the phase-plane one-to-one onto itself. To relate

† This work was performed within a project of the Sonderforschungsbereich 65 Darmstadt-Frankfurt.

0305-4470/79/040451+07$01.00

phase-plane functions $f(x, p)$ to operators we use the correspondence based upon symmetric ordering introduced by Cahill and Glauber (1969) (Weyl correspondence), which is outlined in § 2. These unitary transformations, explicitly defined in § 3, can be used to determine the eigenvalues of a large class of Hamiltonians (e.g. $H(X, P) = \frac{1}{2m}(P^2 + A|X|^\nu)$, A, $\nu > 0$), which will be discussed in § 4.

2. Weyl correspondence

Let us begin by establishing a relation between operators on the Hilbert space $\mathcal{H}^{(1)}$ of one particle without spin† and functions $f(x, p)$ on the (x, p) plane. Following Cahill and Glauber (1969) we define the Hermitian operator

$$T(\alpha) = 2D(\alpha)(-1)^{a^+a}D(-\alpha) \tag{2.1}$$

where $D(\alpha)$ is the displacement operator, introduced by Weyl (1950)

$$D(\alpha) = \exp(\alpha a^+ - a^* a), \qquad \alpha \text{ complex number} \tag{2.2}$$

and $(-1)^{a^+a}$ the parity operator

$$\begin{aligned}(-1)^{a^+a}P(-1)^{a^+a} &= -P\\ (-1)^{a^+a}X(-1)^{a^+a} &= -X.\end{aligned} \tag{2.3}$$

The operators $T(\alpha)$ possess the same type of completeness as do the unitary operators $D(\alpha)$ (Cahill and Glauber 1969)

$$\mathrm{Tr}[T(\alpha)T(\beta)] = \pi\delta^{(2)}(\alpha - \beta) = \mathrm{Tr}[D(-\alpha)D(\beta)]. \tag{2.4}$$

Therefore we may expand any Hilbert–Schmidt‡ operator F in the form ($\alpha = (2\hbar)^{-1/2}(\lambda x + \mathrm{i}\lambda^{-1}p)$, λ real parameter, different from zero)

$$F = \int (\mathrm{d}^2\alpha/\pi) f_a(x, p) T(\alpha) \tag{2.5a}$$

$$F = \int (\mathrm{d}^2\alpha/\pi) f_b(x, p) D(-\alpha) \tag{2.5b}$$

where the functions $f(x, p)$, which are given by the traces

$$f_a(x, p) = \mathrm{Tr}[FT(\alpha)] \tag{2.6a}$$

$$f_b(x, p) = \mathrm{Tr}[FD(\alpha)] \tag{2.6b}$$

are unique and square-integrable

$$\int \frac{\mathrm{d}^2\alpha}{\pi} |f(x, p)|^2 = \mathrm{Tr}[F^+F]. \tag{2.7}$$

† To be more precise $\mathcal{H}^{(1)}$ is a representation space, carrying an irreducible unitary representation of the Heisenberg–Weyl group, the corresponding Lie algebra of which is generated by the operators a, a^+ and 1, satisfying $[a, a^+] = 1$.

‡ We shall say that an operator is an Hilbert–Schmidt operator if its Hilbert–Schmidt norm $\|F\| = (\mathrm{Tr}\, F^+F)^{1/2}$ is finite.

As was shown by Cahill and Glauber (1969) the correspondence

$$F(X, P)\leftrightarrow f_a(x, p) \tag{2.8}$$

is based upon the concept of symmetric ordering of operators and is called Weyl correspondence in the literature. Its advantage is that it can be used for a much larger class of operators than is the class of Hilbert–Schmidt operators, for example

$$a\leftrightarrow\alpha \tag{2.9a}$$

$$a^+\leftrightarrow\alpha^* \tag{2.9b}$$

$$\tfrac{1}{2}(a^+a+aa^+)\leftrightarrow|\alpha|^2 \tag{2.9c}$$

$$H(X, P)=\tfrac{1}{2m}P^2+V(X)\leftrightarrow h(x, p)=\tfrac{1}{2m}p^2+V(x) \tag{2.9d}$$

$$T(\beta)\leftrightarrow\pi\delta^{(2)}(\alpha-\beta). \tag{2.9e}$$

3. Definition of unitary transformations

The class of Hilbert–Schmidt operators $|F)$† spans a Hilbert space $\mathscr{H}^{(2)}$, if one uses the following inner product

$$(F|G)=\mathrm{Tr}[F^+G]. \tag{3.1}$$

The vectors $|\alpha)\equiv|T(\alpha))$—though not elements of $\mathscr{H}^{(2)}$‡—form an orthonormal system in the sense that any vector $|F)\in\mathscr{H}^{(2)}$ can be expanded (see equation (2.5a)) as

$$|F)=\int\frac{\mathrm{d}^2\alpha}{\pi}(\alpha|F)|\alpha)=\int\frac{\mathrm{d}^2\alpha}{\pi}f_a(x, p)|\alpha) \tag{3.2}$$

with

$$\int\frac{\mathrm{d}^2\alpha}{\pi}|f_a(x, p)|^2<\infty. \tag{3.3}$$

Let us now define the following linear operator U on $\mathscr{H}^{(2)}$

$$U|\alpha)=|\bar{\alpha}) \tag{3.4}$$

where $\bar{\alpha}=\bar{\alpha}(x, p)$ is a bijective canonical transformation, i.e. a mapping of the phase-plane (x, p) one-to-one *onto* itself, with

$$\frac{\partial(x, p)}{\partial(\bar{x}, \bar{p})}=1 \tag{3.5a}$$

or equivalently

$$\mathrm{d}^2\alpha=\mathrm{d}^2\bar{\alpha} \tag{3.5b}$$

U is defined on the whole space $\mathscr{H}^{(2)}$ and is a mapping *onto* $\mathscr{H}^{(2)}$. Obviously there exists the adjoint operator U^+ of U which is defined on the whole space $\mathscr{H}^{(2)}$ and is a mapping

† In this section we use a 'Dirac notation' to emphasise that we regard the operators F as elements of a linear space.
‡ The vectors $|\alpha)$ are Dirac 'kets' referring to the space $\mathscr{H}^{(2)}$ in the same sense as being e.g. the eigenkets $|p\rangle$ of the momentum operator P Dirac vectors referring to $\mathscr{H}^{(1)}$.

onto $\mathscr{H}^{(2)}$ as well. Now U^+ is isometric:

$$
\begin{aligned}
(U^+F|U^+G) &= \int \frac{d^2\alpha}{\pi}(U^+F|\alpha)(\alpha|U^+G) \\
&= \int \frac{d^2\alpha}{\pi}(F|U\alpha)(U\alpha|G) \\
&= \int \frac{d^2\bar{\alpha}}{\pi}(F|\bar{\alpha})(\bar{\alpha}|G) = (F|G).
\end{aligned} \tag{3.6}
$$

Therefore—together with the above mentioned properties of U and U^+—it follows that U and U^+ are unitary operators on $\mathscr{H}^{(2)}$.

As a trivial example we take the following linear transformation

$$\bar{\alpha} = \exp(i\phi)\alpha \tag{3.7}$$

or

$$\bar{x} = \cos\phi x - \lambda^{-2}\sin\phi p \tag{3.7a}$$

$$\bar{p} = \lambda^2 \sin\phi + \cos\phi p. \tag{3.7b}$$

Equation (3.7) describes a rigid rotation of the phase plane about an angle ϕ, which is obviously a bijective canonical transformation. It holds

$$
\begin{aligned}
|\bar{X}) &= U|X) \\
&= \int \frac{d^2\alpha}{\pi}\frac{(2\hbar)^{1/2}}{2\lambda}(\alpha+\alpha^*)U|\alpha) \\
&= \int \frac{d^2\bar{\alpha}}{\pi}\frac{(2\hbar)^{1/2}}{2\lambda}(\exp(-i\phi)\bar{\alpha}+\exp(i\phi)\bar{\alpha}^*)|\bar{\alpha}) \\
&= \cos\phi|X)+\lambda^{-2}\sin\phi|P)
\end{aligned} \tag{3.8a}
$$

and analogue

$$|\bar{P}) = -\lambda^2\sin\phi|X)+\cos\phi|p). \tag{3.8b}$$

4. Exact eigenvalues of Hamiltonians

We want to show now how the general formalism introduced in the two preceeding sections can be applied to solve concrete physical problems. First we note that the eigenvalue problem of the number operator $N = a^+a$ is completely known:

$$
\begin{aligned}
N|n\rangle &= n|n\rangle \\
F(N)|n\rangle &= F(n)|n\rangle
\end{aligned}
\qquad n = 0, 1, 2, \ldots. \tag{4.1}
$$

To find the operator $F(N)$ corresponding to a given function $f(|\alpha|^2)$ by symmetric ordering (Weyl correspondence; see equations (2.5a) and (2.8)), we first define the

Laplace transform $\omega(s)$ of $f(|\alpha|^2)$†

$$\omega(s)=\int_0^\infty \mathrm{d}(|\alpha|^2)\exp(-s|\alpha|^2)f(|\alpha|^2) \tag{4.2a}$$

$$f(|\alpha|^2)=\frac{1}{2\pi \mathrm{i}}\int_{x-\mathrm{i}\infty}^{x+\mathrm{i}\infty}\mathrm{d}s\exp(s|\alpha|^2)\omega(s) \qquad s=x+\mathrm{i}y \tag{4.2b}$$

and use now the following formula (Cahill and Glauber 1969):

$$\int\frac{\mathrm{d}^2\alpha}{\pi}\exp(s|\alpha|^2)T(\alpha)=\frac{1}{1-s/2}\left(\frac{1+s/2}{1-s/2}\right)^N. \tag{4.3}$$

Thus we find

$$\begin{aligned}F(N)&=\int\frac{\mathrm{d}^2\alpha}{\pi}f(|\alpha|^2)T(\alpha)\\&=\int\frac{\mathrm{d}^2\alpha}{\pi}\left[\frac{1}{2\pi\mathrm{i}}\int_{x-\mathrm{i}\infty}^{x+\mathrm{i}\infty}\mathrm{d}s\exp(s|\alpha|^2)\omega(s)\right]T(\alpha)\\&=\frac{1}{2\pi\mathrm{i}}\int_{x-\mathrm{i}\infty}^{x+\mathrm{i}\infty}\frac{\mathrm{d}s}{1-s/2}\left(\frac{1+s/2}{1-s/2}\right)^N\omega(s)\end{aligned} \tag{4.4}$$

which states the following:

The eigenvalues $F(n)$ of the operator $F(N)$—corresponding to the function $f(|\alpha|^2)$ by symmetric ordering— are

$$F(n)=\frac{1}{2\pi\mathrm{i}}\int_{x-\mathrm{i}\infty}^{x+\mathrm{i}\infty}\frac{\mathrm{d}s}{1-s/2}\left(\frac{1+s/2}{1-s/2}\right)^n\omega(s) \qquad n=0,1,2,\ldots \tag{4.5}$$

with $\omega(s)$ given by equation (4.2*a*).

Evaluating the integral (4.5) we find

$$F(n)=\frac{2(-1)^n}{n!}\frac{\mathrm{d}^n}{\mathrm{d}s^n}((2+s)^n\omega(s))_{s=2} \qquad n=0,1,2,\ldots. \tag{4.6}$$

Now the usually given physical Hamiltonians do not have the functional dependence $F(N)$—except the linear harmonic oscillator. But for a certain class of operators H we can use a unitary transformation U to relate a given Hamiltonian $H=H(a,a^+)$ from this class to an operator $\bar{H}=\bar{H}(N)$ as follows:

$$\begin{aligned}U|H)&=\int\frac{\mathrm{d}^2\alpha}{\pi}h(\alpha,\alpha^*)U|\alpha)=\int\frac{\mathrm{d}^2\alpha}{\pi}h(\alpha,\alpha^*)|\bar{\alpha})\\&=\int\frac{\mathrm{d}^2\bar{\alpha}}{\pi}\bar{h}(|\bar{\alpha}|^2)|\bar{\alpha})=|\bar{H})\end{aligned} \tag{4.7a}$$

with U defined by equations (3.4) and (3.5), especially holds

$$UU^+=U^+U=1 \quad \text{on } \mathscr{H}^{(2)}. \tag{4.7b}$$

Because of equations (4.7) H and $\bar{H}$ are unitarily equivalent and have equal eigenvalues. To determine therefore the eigenvalues of H we notice that the curves of

† In the following it is assumed that the mathematical statements leading to equation (4.6) are well-defined, which is of course a condition upon the functions f and F.

constant value of the Hamiltonian function $\bar{h}(|\bar{\alpha}|^2)$ are circles around the origin in an $\bar{\alpha}$ phase-plane. We can now state the following:

A class of Hamiltonians, whose eigenvalues can exactly be calculated by equation (4.5), consists of operators H, whose curves of constant value of the corresponding Hamiltonian function $h(\alpha, \alpha^*)$ are the pictures in the α plane of concentric circles in the $\bar{\alpha}$ plane by a bijective canonical transformation $\alpha = \alpha(\bar{\alpha}, \bar{\alpha}^*)$.

To construct the unknown Hamiltonian function $\bar{h}(|\bar{\alpha}|^2)$ for a given Hamiltonian function $h(x, p)$, we proceed along the lines of classical physics, and use the action variable $\mathscr{F}(E)$:

$$\mathscr{F}(E) = \frac{1}{2\pi\hbar}\int_{h(x,p)=E} p(x; E)\,\mathrm{d}x = \frac{1}{2\hbar}(\lambda^2\bar{x}^2 + \lambda^{-2}\bar{p}^2) = |\bar{\alpha}|^2. \tag{4.8}$$

Equation (4.8) defines $|\bar{\alpha}|^2$ as a function of E, which relation gives us the desired function $\bar{h}$ by inversion

$$E = \bar{h}(|\bar{\alpha}|^2). \tag{4.9}$$

For illustration let us now calculate the eigenvalues of the following class of Hamiltonians:

$$H(X, P) = \tfrac{1}{2m}(P^2 + a^{\frac{1}{2}(\nu+2)}|X|^\nu) \qquad a, \nu > 0. \tag{4.10}$$

The paths in the (x, p)-plane defined by $p^2 + a^{\frac{1}{2}(\nu+2)}|x|^\nu = 2mE$ are closed curves, and are the pictures of concentric circles by a bijective canonical transformation. We find

$$\begin{aligned}|\bar{\alpha}|^2 = \mathscr{F}(E) &= \frac{1}{2\pi\hbar}\int_{h(x,p)=E} \mathrm{d}x\, (2mE - a^{\frac{1}{2}(\nu+2)}|x|^\nu)^{1/2} \\ &= \frac{4(2mE)^{1/2}}{\hbar}\left(\frac{2mE}{a^{\frac{1}{2}(\nu+2)}}\right)^{\nu^{-1}}\frac{1}{2\pi}\int_0^1 \mathrm{d}q\, (1-q^\nu)^{1/2}\end{aligned} \tag{4.11}$$

or

$$E = \bar{h}(|\bar{\alpha}|^2) = \frac{a}{2m}\left(\frac{\hbar|\bar{\alpha}|^2}{4b_\nu}\right)^{2\nu/(\nu+2)} \tag{4.12a}$$

with

$$b_\nu = \frac{1}{2\pi}\int_0^1 \mathrm{d}q\, (1-q^\nu)^{1/2}. \tag{4.12b}$$

Laplace transformation of equation (4.12a) yields

$$\omega(s) = \frac{a}{2m}\left(\frac{\hbar}{4b_\nu}\right)^{2\nu/(\nu+2)}\Gamma\left(1 + \frac{2\nu}{\nu+2}\right)s^{-(1+2\nu/(\nu+2))}. \tag{4.13}$$

Now we can use equation (4.6) and get for the eigenvalues $E^{(\nu)}(n)$ of the Hamiltonian (4.10):

$$E^{(\nu)}(n) = \frac{a}{m}\left(\frac{\hbar}{4b_\nu}\right)^{2\nu/(\nu+2)}\Gamma[1 + 2\nu/(\nu+2)]\frac{(-1)^n}{n!}\frac{\mathrm{d}^n}{\mathrm{d}s^n}\left(\frac{(2+s)^n}{s^{1+2\nu/(\nu+2)}}\right)_{s=2}. \tag{4.14}$$

5. Conclusions

Using the Weyl correspondence between operator functions $F(X, P)$ and c-number functions $f(x, p)$ we have succeeded in defining non-linear unitary transformations with the help of bijective canonical transformations. By these unitary transformations we were able to derive a formula for the exact eigenvalues $E(n)$ of a large class of Hamiltonians $H(X, P)$ (see equation (4.5)):

$$E(n) = \frac{1}{2\pi\mathrm{i}} \int_{x-\mathrm{i}\infty}^{x+\mathrm{i}\infty} \frac{\mathrm{d}s}{1-s/2}\left(\frac{1+s/2}{1-s/2}\right)^n \omega(s)$$

$$= \frac{1}{2\pi\mathrm{i}} \int_{x-\mathrm{i}\infty}^{x+\mathrm{i}\infty} \frac{\mathrm{d}s}{(1-s^2/4)^{1/2}} \exp[(n+\tfrac{1}{2}) \ln(1+s/2)/(1-s/2)]\omega(s). \tag{5.1}$$

By expanding the square root and the logarithmic function in the exponent of the integrand we arrive in a first step at the well-known WKB approximation, often used in the literature in deriving energy eigenvalues:

$$E(n) \approx \frac{1}{2\pi\mathrm{i}} \int_{x-\mathrm{i}\infty}^{x+\mathrm{i}\infty} \mathrm{d}s \exp[(n+\tfrac{1}{2})s]\omega(s) = \bar{h}(|\bar{\alpha}|^2 = n+\tfrac{1}{2}) = E^{\mathrm{WKB}}(n). \tag{5.2}$$

Thus we are able to test the WKB approximation (5.2) by the exact values (5.1) for the class of systems, described in § 4.

Our further studies shall be to extend formula (5.1) to other classes of potentials such as $V(x) = (x^2 - 1)^2$, the eigenvalues of which are important in the theory of structural phase transitions. The eigenvalues of potentials like $V(x) = (x^2 - 1)^2$ will be discussed in a further paper.

Acknowledgments

The author is grateful to Professor E Fick for valuable advice and to Professor G Sauermann for helpful discussions.

References

Cahill K E and Glauber R J 1969 *Phys. Rev.* **177**II 1857–81, 1882–1902
Dirac P A M 1958 *Quantum Mechanics* 4th ed (London: Oxford University Press) 103–7
Goldstein H 1963 *Klassische Mechanik* (Frankfurt: Akademische Verlagsgesellschaft) 263–348
Kramer P, Moshinsky M and Seligman T H 1978 *J. Math. Phys.* **19** 683–93
Weyl H 1950 *The Theory of Groups and Quantum Mechanics* (New York: Dover) 272–6