The Heisenberg−Weyl Algebra on the Circle and a Related Quantum Mechanical Model for Hindered Rotation†

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We discuss a periodic variant of the Heisenberg−Weyl algebra, associated with the group of translations and modulations on the circle. Our study of uncertainty minimizers leads to a periodic version of canonical coherent states. Unlike the canonical, Cartesian case, there are states for which the uncertainty product associated with the generators of the algebra vanishes. Next, we explore the supersymmetric (SUSY) quantum mechanical setting for the uncertainty-minimizing states and interpret them as leading to a family of "hindered rotors". Finally, we present a standard quantum mechanical treatment of one of these hindered rotor systems, including numerically generated eigenstates and energies.

I. Introduction

The Heisenberg uncertainty principle is fundamental to quantum mechanics since it precludes the existence of precise simultaneous measurements of position and momentum.[1] It also gives a hint of which quantum states are most compatible with classical mechanics.[2−9] In these states, the uncertainty product of the kinematic variables equals the expectation value of the imaginary part of their commutator. For the case of position and momentum operators $\hat{x}$ and $\hat{p}$ (or when setting $\hbar \equiv 1$, $\hat{x}$, and the wavenumber operator, $\hat{k}$), these operators, along with the identity, $\hat{I}$, observe the so-called canonical commutation relations associated with the Heisenberg−Weyl Lie algebra.[3,5,6] The uncertainty minimizers for this case are the "canonical" coherent states which result from requiring that the uncertainty product of the position and momentum variances to attain the absolute minimum. Various aspects of the coherent states are best dealt with using the complexified Lie algebra,[5] containing the canonical raising and lowering operators. The raising and lowering operators also appear when factoring the harmonic oscillator Hamiltonian.[2] Indeed, the factorization approach to quantum mechanics provides a rich viewpoint that is central to much research in modern quantum theory (the so-called "supersymmetric" or SUSY quantum mechanics).[10−12] In this paper, we are interested in exploring a periodic variant of the Heisenberg−Weyl algebra, which leads to a new approach to the quantum mechanics of hindered rotation. There is, of course, a connection to the harmonic oscillator since in many systems of physical interest, the dynamics of a hindered rotor are "locally" harmonic. That is, for small oscillations, the hindering potential is harmonic. Such systems occur in many guises, for example, the rotation of methyl or other end groups in organic chemistry, the dynamics of particles in multiple barriers, surface motion of absorbed atoms or molecules, electrons in solids, and so forth. Typically, one assumes a periodic potential when modeling many such systems. Here, we shall arrive at such a model by considering an appropriate variant of the Heisenberg−Weyl algebra, which takes into account that the spectrum of the position operator is no longer the entire real line but rather a bounded interval of angles. In brief, we shall develop a periodic variant of the Heisenberg−Weyl algebra and explore the consequences.

The remainder of this paper is organized as follows. In section II, we find operators that incorporate the periodic nature of planar rotor dynamics and locally approximate the Heisenberg−Weyl algebra. This involves replacing the operators $\hat{x}$, $\hat{k}$, and $\hat{I}$ by new operators. The resulting algebra will be explored in detail, including its relation to the standard Heisenberg−Weyl algebra. We also derive constrained minimum uncertainty states and compare them to canonical coherent states. In section III, we consider the hindered rotor and related systems using the SUSY quantum mechanics approach. The parallels and differences between the hindered rotor and the harmonic oscillator are discussed in detail. In section IV, we consider excited states of the new hindered rotor, both analytically and numerically. In the former case, we examine the quantization conditions arising from the requirements of periodicity and continuity of the solutions. Finally, in section V, we present our conclusions and indicate some avenues of future research.

II. A Periodic Generalization of the Heisenberg−Weyl Algebra

We begin with two observations regarding the one-dimensional hindered rigid rotor in relation to the harmonic oscillator. We denote the position operator by $\hat{x}$ and the momentum operator by $\hat{p}$. In the so-called coordinate representation, they act by multiplication and differentiation on any sufficiently

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regular square integrable wave function ψ, $\hat{x}\psi(x) = x\psi(x)$ and $\hat{p}\psi(x) = -i\hbar d\psi(x)/dx$. Denoting the "wave number" operator by $\hat{k} = \hat{p}/\hbar$ and the identity by $\hat{I}$, we have the commutation relations[5]

$$[\hat{x}, \hat{k}]\psi \equiv (\hat{x}\hat{k} - \hat{k}\hat{x})\psi = i\psi \tag{II.1}$$

and

$$[\hat{x}, \hat{I}]\psi = [\hat{k}, \hat{I}]\psi = 0 \tag{II.2}$$

Here ψ is assumed to be in the domains of the operator products $\hat{x}\hat{k}$ and $\hat{k}\hat{x}$.

A state ψ, that is, a normalized wave function, is, in our interpretation, closest to classical if it minimizes the Heisenberg uncertainty product $\Delta\hat{x}\Delta\hat{k} \equiv (\langle(\hat{x} - \langle\hat{x}\rangle)^2\rangle\langle(\hat{k} - \langle\hat{k}\rangle)^2\rangle)^{1/2}$ for each fixed expectation value of position and wavenumber, $\langle\hat{x}\rangle = \langle\psi|\hat{x}|\psi\rangle$ and $\langle\hat{k}\rangle = \langle\psi|\hat{k}|\psi\rangle$. For the convenient minimization of the Heisenberg uncertainty product, we define a lowering operator which we adjust to any pair of expectation values $\langle\hat{x}\rangle$ and $\langle\hat{k}\rangle$ of a given state ψ according to

$$\hat{a} = \frac{1}{\sqrt{2}}(\hat{x} - \langle\hat{x}\rangle + i\sigma^2(\hat{k} - \langle\hat{k}\rangle)) \tag{II.3}$$

where σ is a proportionality factor.

The so-called canonical coherent states are precisely the ones annihilated by $\hat{a}$

$$\hat{a}\psi_0 = 0 \tag{II.4}$$

or

$$\frac{1}{\sqrt{2}}\left[\sigma^2\left(\frac{d}{dx} - i\langle\hat{k}\rangle\right) + (x - \langle\hat{x}\rangle)\right]\psi_0(x) = 0 \tag{II.5}$$

The solution to this first-order differential equation is

$$\psi_0(x) = \psi_0(0)e^{-(x-\langle\hat{x}\rangle)^2/2\sigma^2}e^{i\langle\hat{k}\rangle x}e^{\langle\hat{x}\rangle^2/2\sigma^2} \tag{II.6}$$

which is recognized as the Heisenberg−Weyl coherent state.[3,5,6,9] The magnitude of the constant $\psi_0(0)$ is determined by the normalization condition

$$||\psi_0||^2 = \int_{\mathbb{R}}|\psi_0(x)|^2 dx = 1$$

When choosing the coordinate origin as the expectation value for position and momentum in phase space and a convenient energy scale, then ψ_0 is also the ground state for the simple harmonic oscillator Hamiltonian

$$\hat{H}_{HO} = \frac{1}{2}(\hat{x}^2 + \hat{k}^2) \tag{II.7}$$

Factorizing the harmonic oscillator Hamiltonian

$$\hat{H}_{HO} = \hat{a}^+\hat{a} + \frac{1}{2} = \hat{a}\hat{a}^+ - \frac{1}{2} \tag{II.8}$$

is achieved with the corresponding raising operator[2]

$$\hat{a}^+ = \frac{1}{\sqrt{2}}(\hat{x} - i\hat{k}) \tag{II.9}$$

which is the adjoint of $\hat{a}$; therefore, $\hat{a}^+ = \hat{a}^\dagger$.

We now introduce a periodic variant, appropriate to the hindered rotor, that is generated by the Hermitian operators $\hat{k}_\varphi$, $\hat{s}$, and $\hat{c}$, which act in the coordinate representation on a sufficiently regular 2π-periodic function ψ by

$$\hat{k}_\varphi\psi(\varphi) = -i\frac{d}{d\varphi}\psi(\varphi) \tag{II.10}$$

$$\hat{s}\psi(\varphi) = \sin\varphi\psi(\varphi) \tag{II.11}$$

$$\hat{c}\psi(\varphi) = \cos\varphi\psi(\varphi) \tag{II.12}$$

We evaluate the relevant commutators

$$[\hat{s}, \hat{k}_\varphi]\psi = i\hat{c}\psi \tag{II.13}$$

$$[\hat{c}, \hat{k}_\varphi]\psi = -i\hat{s}\psi \tag{II.14}$$

and

$$[\hat{s}, \hat{c}]\psi = 0 \tag{II.15}$$

If ψ is concentrated in the neighborhood of $\varphi = 0$, then $\hat{k}_\varphi$, $\hat{s}$, and $\hat{c}$ approximate $\hat{k}$, $\hat{x}$, $\hat{I}$ since then, in the coordinate representation

$$\hat{k}_\varphi = -i\frac{d}{d\varphi} \quad \hat{s} \approx \hat{\varphi} \quad \text{and} \quad \hat{c} \approx \hat{I} \tag{II.16}$$

and the commutation relations become

$$[\hat{s}, \hat{k}_\varphi]\psi \approx i\psi \tag{II.17}$$

$$[\hat{c}, \hat{k}_\varphi]\psi \approx 0 \tag{II.18}$$

and

$$[\hat{s}, \hat{c}]\psi = 0 \tag{II.19}$$

In the following, we wish to discuss minimizers for the uncertainty product $\Delta\hat{s}\Delta\hat{k}_\varphi$, for fixed expected values $\langle\hat{s}\rangle$, $\langle\hat{c}\rangle$, and $\langle\hat{k}_\varphi\rangle$. We want to investigate in which sense these minimizers resemble the ones associated with the Heisenberg−Weyl algebra. We have chosen $\hat{s}$, corresponding to one coordinate of the circle, to take the place of the position operator. In general, any one-dimensional component of the coordinate operator

$\cos(\varphi_0)\hat{s} + \sin(\varphi_0)\hat{c}$ with some angle $\varphi_0 \in [0,2\pi]$ would be possible (along with the companion operator $\sin(\varphi_0)\hat{s} + \cos(\varphi_0)\hat{c}$); see the comments further below.

Apart from the fact that we fix the expected value for three operators $\hat{s}$, $\hat{c}$, and $\hat{k}_\varphi$ instead of just two, it is important to note that there is a fundamental difference in the behavior of $\Delta\hat{s}\Delta\hat{k}_\varphi$ compared to $\Delta\hat{x}\Delta\hat{k}$. This is due to the fact that $\hat{k}_\varphi$ has normalizable eigenvectors, and thus when ψ_n satisfies $\hat{k}_\varphi\psi_n = n\psi_n$, we obtain $\Delta\hat{k}_\varphi = 0$, and the uncertainty product vanishes. These eigenstates form an orthonormal basis, which is of value for studying the planar, free rigid rotor and its perturbations.

Nevertheless, the vanishing uncertainty product only occurs in these eigenstates, and then, $\langle\hat{s}\rangle = 0$ and $\langle\hat{c}\rangle = 0$. We want to investigate the general case in which these expected values can be nonzero as well.

Suppose we want to minimize $\Delta\hat{s}\Delta\hat{k}_\varphi$ among all of the states $\psi_0^{(s)}$ for which the quantum system has a fixed expected value $\langle\hat{s}\rangle$, $\langle\hat{c}\rangle$, and $\langle\hat{k}_\varphi\rangle$. This means that the expected position on the circle has a bias, and so does the expected wavenumber.

We claim a lower bound for the uncertainty product $\Delta\hat{s}\Delta\hat{k}_\varphi$, which is assumed for a minimizer ψ that is unique up to an overall unimodular constant.

To see this, we note that if the inequalities

$$\langle\psi_0^{(s)}|(\hat{s} - \langle\hat{s}\rangle)^2|\psi_0^{(s)}\rangle\langle\psi_0^{(s)}|(\hat{k}_\varphi - \langle\hat{k}_\varphi\rangle)^2|\psi_0^{(s)}\rangle \geq |\langle\psi_0^{(s)}|(\hat{s} - \langle\hat{s}\rangle)(\hat{k}_\phi - \langle\hat{k}_\varphi\rangle)|\psi_0^{(s)}\rangle|^2 \geq \frac{1}{4}(\langle\psi_0^{(s)}|\mathrm{i}[\hat{s} - \langle\hat{s}\rangle, \hat{k}_\phi - \langle\hat{k}_\varphi\rangle]|\psi_0^{(s)}\rangle)^2 = \frac{1}{4}(\langle\psi_0^{(s)}|\hat{c}|\psi_0^{(s)}\rangle)^2 \quad \text{(II.20)}$$

are saturated, then equality holds in the above application of the Cauchy−Schwarz inequality and

$$-\beta(\hat{s} - \langle\hat{s}\rangle)|\psi_0^{(s)}\rangle = -\mathrm{i}(\hat{k}_\varphi - \langle\hat{k}_\varphi\rangle)|\psi_0^{(s)} \quad \text{(II.21)}$$

where β is a necessarily real constant.

The solution to this ordinary differential equation is

$$\psi_0^{(s)}(\varphi) = \psi_0^{(s)}(0)\mathrm{e}^{\beta\cos\varphi + \beta\langle\hat{s}\rangle\varphi + \mathrm{i}\langle\hat{k}_\varphi\rangle\varphi} \quad \text{(II.22)}$$

We next observe that since β and $\langle\hat{s}\rangle$ are real ($\hat{s}$ is Hermitian), the periodicity requirement implicit in the fact that ψ is in the domain of $\hat{k}_\varphi$ forces $\langle\hat{s}\rangle \equiv 0$ and

$$\langle\hat{k}_\varphi\rangle = n \qquad n = 0, \pm1, \pm2, ... \quad \text{(II.23)}$$

so the result is

$$\psi_n^{(s)}(\varphi) = \psi_n^{(s)}(0)\mathrm{e}^{\beta\cos\varphi + \mathrm{i}n\varphi} \quad \text{(II.24)}$$

Note that unlike the canonical $\hat{x}$,$\hat{k}$ case, β could be positive or negative, depending on the constraint for $\hat{c}$. This is because the normalization condition

$$\int_0^{2\pi} |\psi_0^{(s)}(\varphi)|^2 \mathrm{d}\varphi = 1 \quad \text{(II.25)}$$

can be satisfied regardless of the sign of β.

In addition, for the periodic coherent states, the eigenvalue associated with each coherent state is $\langle s\rangle + \mathrm{i}\langle k_\varphi\rangle \equiv \mathrm{i}n$ since $\langle s\rangle$ must be 0. This means the periodic coherent states are indexed by $\langle k_\varphi\rangle$ and by β.

We claim that there is a unique β for each value of $\langle\hat{c}\rangle$. To verify this, we use a shorthand notation for un-normalized expressions $\langle\langle\hat{c}\rangle\rangle = \int_{-\pi}^{\pi} \cos\varphi\, \mathrm{e}^{2\beta\cos\varphi}\mathrm{d}\varphi$, $\langle\langle\hat{I}\rangle\rangle = \int_{-\pi}^{\pi} \mathrm{e}^{2\beta\cos\varphi}\mathrm{d}\varphi$, and similar for other operators. It is sufficient to show that $\langle\hat{c}\rangle = \langle\langle\hat{c}\rangle\rangle/\langle\langle\hat{I}\rangle\rangle$ is strictly increasing in β. Indeed, we have

$$\frac{\mathrm{d}}{\mathrm{d}\beta}\langle\hat{c}\rangle = 2\frac{\langle\langle\hat{c}^2\rangle\rangle\langle\langle\hat{I}\rangle\rangle - (\langle\langle\hat{c}\rangle\rangle)^2}{(\langle\langle\hat{I}\rangle\rangle)^2}$$

and the Cauchy−Schwarz inequality shows that the numerator is strictly positive because

$$\langle\langle\hat{c}^2\rangle\rangle\langle\langle\hat{I}\rangle\rangle > (\langle\langle\hat{c}\hat{I}\rangle\rangle)^2$$

The inequality is strict because the inner product $\langle\langle\hat{c}\hat{I}\rangle\rangle$ is not between collinear vectors.

If the uncertainty inequality eq II.20 is saturated, then inserting eq II.21 gives

$$(\Delta\hat{s})^2 = \frac{\langle\psi_0^{(s)}|\hat{c}|\psi_0^{(s)}\rangle}{2\beta}$$

Near $\varphi = 0$, $\cos\varphi - 1 \approx -\varphi^2/2$; therefore, we obtain (locally near $\varphi = 0$)

$$\psi_0^{(s)}(\varphi) \approx \psi_n^{(s)}(0)\mathrm{e}^{\beta-(\beta\varphi^2/2)+\mathrm{i}n\varphi} \quad \text{(II.26)}$$

Moreover, if the constraint is $\langle\psi_0^{(s)}|\hat{c}|\psi_0^{(s)}\rangle \approx 1$, then the state is concentrated near $\varphi = 0$, β is large, and

$$(\Delta\hat{s})^2 \approx \frac{1}{2\beta}$$

is small. This is therefore an approximation of the Cartesian, canonical coherent states. The likeness is strongest for large $\beta > 0$, but we stress that for the periodic coherent states discussed here, $\beta < 0$ is also allowed, leading to a locally inverse Gaussian behavior. The value $\beta = 0$ is permitted if $\hat{c}$ has the expected value of 0. In that case, one simply obtains again the eigenstates of the standard, planar rigid rotor. Finally, we observe that the periodic canonical states can be viewed as indexed by $\langle k_\varphi\rangle$ and $\beta = (1/2)\langle c\rangle/(\Delta s)^2$. That is, there are now three operators (rather than two as for the Cartesian case), albeit $\langle c\rangle$ and Δs combine to yield a single index. The parameter β acts to “dictate” the circle.

Before considering the quantum dynamics of the hindered rotor, we briefly mention that other uncertainty products can be minimized in the same way, for example, $\Delta\hat{c}\Delta\hat{k}_\varphi$ or $\cos(\phi)\hat{s} + \sin(\phi)\hat{c}$ with some angle $\phi \in [0,2\pi]$.

Following the same strategy as before for $\Delta\hat{c}\Delta\hat{k}_\varphi$, we obtain a minimizer $\psi_0^{(c)}$ which satisfies

$$\psi_0^{(c)}(\varphi) = \psi_0^{(c)}(0)\mathrm{e}^{\gamma\sin\varphi + \gamma\langle\hat{c}\rangle\varphi + \mathrm{i}\langle\hat{k}_\varphi\rangle\varphi} \quad \text{(II.27)}$$

with some real parameter γ. In this case, we require $\langle\hat{c}\rangle \equiv 0$ for a periodic solution, as well as $\langle\hat{k}_\varphi\rangle \equiv n$, $n = 0, \pm 1, \ldots$. This gives

$$\psi_0^{(c)}(n,\varphi) = \psi_{n,0}^{(c)}(0)e^{\gamma \sin\varphi + in\varphi} \tag{II.28}$$

In contrast to the minimizers for $\Delta\hat{s}\Delta\hat{k}_\varphi$, these states are concentrated at $\varphi = \pm\pi/2$, unless $\gamma = 0$, in which case, we recover the free planar rotor states again.

We next consider

$$S = \sum_{n=-\infty}^{\infty} \psi_n^*(\varphi')\psi_n(\varphi) \tag{II.29}$$

where $\psi_n(\varphi)$ is the nth periodic coherent state

$$\psi_n(\varphi) = \frac{1}{N_n}e^{\beta\cos\varphi + in\varphi} \qquad n = 0, \pm 1, \pm 2, \ldots \tag{II.30}$$

and N_n is the normalization factor. It is explicitly

$$N_n^2 = \int_{-\pi}^{\pi} \psi_n^*(\varphi)\psi_n(\varphi)d\varphi \equiv \int_{-\pi}^{\pi} e^{2\beta\cos\varphi}d\varphi = 2\pi\frac{1}{\pi}\int_0^{\pi} e^{2\beta\cos\varphi}d\varphi = 2\pi I_0(2\beta) \tag{II.31}$$

where I_υ is the υth modified Bessel function of the first kind. Thus, the normalization is independent of the state index, n. It follows that eq II.29 becomes

$$S = \frac{2\pi}{N^2}e^{\beta(\cos\varphi + \cos\varphi')}\sum_{n=-\infty}^{\infty}\frac{e^{in(\varphi-\varphi')}}{2\pi} \tag{II.32}$$

It is then evident that

$$S = \frac{2\pi}{N^2}e^{2\beta\cos\varphi}\delta(\varphi - \varphi') \tag{II.33}$$

which completes the proof. In fact, we observe that the periodic coherent states resulting from the minimization of the pair of operators, $\hat{c}$, $\hat{k}_\varphi$, also satisfy an analogous relation. In this case

$$\psi_n(\varphi) = \frac{1}{N_n}e^{\gamma\sin\varphi + in\varphi} \qquad n = 0, \pm 1, \pm 2, \ldots \tag{II.34}$$

so that eq II.33 now reads

$$S = \frac{2\pi}{N^2}e^{2\gamma\sin\varphi}\delta(\varphi - \varphi') \tag{II.35}$$

In this regard, we expect that expansions using either set of periodic coherent states should prove useful.

It should be obvious that more general combinations of $\hat{c}$ and $\hat{s}$ are also possible.

Finally, we comment on the periodic lowering operators that result from each of the minimizations. We have from eq II.20, for $\langle\hat{s}\rangle = \langle\hat{k}_\varphi\rangle = 0$

$$\hat{A}^{(s)} = \xi(\lambda\hat{s} - \hat{k}_\varphi) \tag{II.36}$$

where ξ is a constant factor. For later convenience, we take $\lambda = -i/(2)^{1/2}$ and $\xi = i$ to obtain

$$\hat{A}^{(s)} = \frac{1}{\sqrt{2}}\left[\sin\varphi + \frac{d}{d\varphi}\right] \tag{II.37}$$

We expect the raising operator to be

$$\hat{A}^{(s)\dagger} = \frac{1}{\sqrt{2}}\left[\sin\varphi - \frac{d}{d\varphi}\right] \tag{II.38}$$

Analogously, the equation

$$\hat{k}_\varphi - \langle\hat{k}_\varphi\rangle|\psi_0^{(c)}\rangle = \alpha(\hat{c} - \langle\hat{c}\rangle)|\psi_0^{(c)}\rangle$$

defines a lowering operator $\hat{A}^{(c)}$, but we shall focus most of our study on $\hat{A}^{(s)}$. We now turn to consider the quantum dynamics of the hindered rotor.

III. Supersymmetric Quantum Dynamics of the Hindered Rotor

The SUSY strategy will be to interpret the minimum uncertainty state, $|\psi_0^{(s)}\rangle$, as the ground state of a quantum dynamical system. The simplest realization of this strategy is to require that $|\psi_0^{(s)}\rangle$ be the ground state of a positive semidefinite Hamiltonian operator with ground-state energy of $E = 0$. Then, in the angular position representation, we require

$$-\frac{d^2}{d\varphi^2}\psi_0^{(s)} = -V(\varphi)\psi_0^{(s)} \tag{III.1}$$

For the ground state corresponding to $\beta = 1$, we have

$$\psi_0^{(s,+)}(\varphi) = \psi_0^{(s,+)}(0)e^{\cos\varphi - 1} \tag{III.2}$$

The "+" superscript denotes the sign of β as positive, and the potential corresponding to this state is denoted by $V_+(\varphi)$. It is easily verified that

$$V_+(\varphi) = \sin^2\varphi - \cos\varphi \tag{III.3}$$

We present a plot of $V_+(\varphi)$ in Figure 1 and observe that it clearly is a potential governing a hindered rotor.[13] We also note that $V_+(\varphi)$ is periodic with a period of 2π. In addition, we could have taken $\beta = -1$, so that

$$\psi_0^{(s,-)}(\varphi) = \psi_0^{(s,-)}(0)e^{-\cos\varphi} \tag{III.4}$$

In general, the SUSY ground state is

$$\psi^{(\pm)} = e^{\mp \int_0^{\varphi} W(\varphi')d\varphi'} \quad \text{(III.5)}$$

The potential associated with $\psi_0^{(s,-1)}$ is

$$V_{-(\varphi)} = \sin^2 \varphi + \cos \varphi \quad \text{(III.6)}$$

We observe that

$$\psi_0^{(s,-)}(\varphi + \pi) = \psi_0^{(s,-)}(0)e^{\cos \varphi} \quad \text{(III.7)}$$

so that $\psi_0^{(s,\pm)}(\varphi)$ and $V_\pm(\varphi)$ are related to one other by a simple translation in φ by an amount $\pm\pi$. Systems of this type are of importance in SUSY quantum mechanics and are known as "self isospectral".[14] We denote the Hamiltonians $H_\pm$, defined as $H_\pm = -(d^2/d\varphi^2) + V_\pm(\varphi)$, where

$$V_+(\varphi \pm \pi) = V_-(\varphi) \quad \text{(III.8)}$$

that is, the two potentials are periodic and related by a simple translation of variables.

To pursue such aspects further, we now formulate our equations within the SUSY framework. The analysis leading to the minimum uncertainty delivers a lowering operator, and this suggests that one solve eq III.1 by a factorization approach. In the supersymmetry approach, we expect to factor the Schrödinger equation in the form[11,12]

$$\left[-\frac{d}{d\varphi} + W(\varphi)\right]\left[\frac{d}{d\varphi} + W(\varphi)\right]\psi = E\psi \quad \text{(III.9)}$$

where $W(\varphi)$ is the superpotential, in terms of which[7,8]

$$V_\pm(\varphi) = W^2(\varphi) \mp \frac{d}{d\varphi}W(\varphi) \quad \text{(III.10)}$$

As is well-known, eq III.5 is the Riccati substitution for the Schrödinger equation, and in this case, we immediately identify $W(\varphi)$ as (compare eq III.7 with eq III.4) eq III.7 with eq III.4.

$$W(\varphi) = \sin \varphi \quad \text{(III.11)}$$

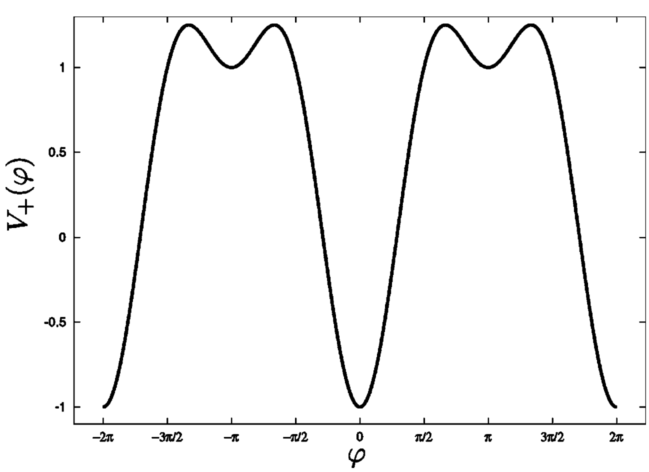

Figure 1. $V_+(\varphi)$ is shown versus φ.

The ground state associated with $V_+(\varphi)$ is then given by solving

$$\left[\frac{d}{d\varphi} + W(\varphi)\right]\psi_0^{(s,+)} = \hat{A}^{(s)}\psi_0^{(s,+)} = 0 \quad \text{(III.12)}$$

or, as before

$$\psi_0^{(s,+)}(\varphi) = \psi_0^{(s,+)}(0)e^{\cos \varphi - 1} \quad \text{(III.13)}$$

The ground state associated with $V_-(\varphi)$ is obtained by solving

$$\left[-\frac{d}{d\varphi} + \sin \varphi\right]\psi_0^{(s,-)} \equiv \hat{A}^{(s)\dagger}\psi_0^{(s,-)} = 0 \quad \text{(III.14)}$$

This gives

$$\psi_0^{(s,-)}(\varphi) = \psi_0^{(s,-)}(0)e^{-\cos \varphi + 1} \quad \text{(III.15)}$$

We also now note that we can factor the hindered rotor Hamiltonians according to

$$\hat{H}_+ = \hat{A}^{(s)\dagger}\hat{A}^{(s)} \quad \text{(III.16)}$$

and

$$\hat{H}_- = \hat{A}^{(s)}\hat{A}^{(s)\dagger} \quad \text{(III.17)}$$

Both $\hat{H}_+$ and $\hat{H}_-$ have zero-eigenvalue ground states. The excited states of $\hat{H}_+$ satisfy

$$\hat{H}_+|\psi_n^{(s,+)}\rangle = E_n|\psi_n^{(s,+)}\rangle \quad \text{(III.18)}$$

We note that

$$\hat{A}^{(s)}\hat{H}_+|\psi_n^{(s,+)}\rangle = E_n\hat{A}^{(s)}|\psi_n^{(s,+)}\rangle \quad \text{(III.19)}$$

However

$$\hat{A}^{(s)}(\hat{H}_+) \equiv \hat{H}_-(\hat{A}^{(s)}) \quad \text{(III.20)}$$

and clearly, $\hat{H}_\pm$ and $\hat{A}^{(s)}$ obey an intertwining relation. We find that

$$\hat{H}_-\hat{A}^{(s)}|\psi_n^{(s,+)}\rangle = E_n\hat{A}^{(s)}|\psi_n^{(s,+)}\rangle \quad \text{(III.21)}$$

Thus

$$\frac{1}{\sqrt{E_n}}\hat{A}^{(s)}|\psi_n^{(s,+)}\rangle = |\psi_n^{(s,-)}\rangle \quad \text{(III.22)}$$

with the same eigenvalue. A similar analysis shows that

$$\hat{H}_-|\psi_n^{(s,-)}\rangle = E_n|\psi_n^{(s,-)}\rangle \quad \text{(III.23)}$$

so that

$$\frac{1}{\sqrt{E_n}}\hat{A}^{(s)\dagger}|\psi_n^{(s,-)}\rangle = |\psi_n^{(s,+)}\rangle \tag{III.24}$$

Clearly, if we can determine the $|\psi_0^{(s,+)}\rangle$, we immediately can generate the $|\psi_0^{(s,-)}\rangle$ states. Unfortunately, the analysis does not enable us to determine either ladder of states without knowledge of the other ladder of states. We shall return later to consider the excited states. (Of course, in the present, periodic case, the states $|\psi_0^{(s,+)}\rangle$ and $|\psi_0^{(s,-)}\rangle$ can be related by translating φ by an amount $\pm\pi$.) For the sake of completeness, we note that a supersymmetric description of the system involves creating a super Hamiltonian

$$\underline{\hat{\mathbf{H}}} = \begin{pmatrix} \hat{A}^{(s)\dagger}\hat{A}^{(s)} & 0 \\ 0 & \hat{A}^{(s)}\hat{A}^{(s)\dagger} \end{pmatrix} \tag{III.25}$$

There are corresponding charge operators, $\hat{Q}$ and $\hat{Q}^\dagger$, given by

$$\underline{\hat{\mathbf{Q}}} = \begin{pmatrix} 0 & 0 \\ \hat{A}^{(s)} & 0 \end{pmatrix} \tag{III.26}$$

and

$$\underline{\hat{\mathbf{Q}}}^\dagger = \begin{pmatrix} 0 & \hat{A}^{(s)\dagger} \\ 0 & 0 \end{pmatrix} \tag{III.27}$$

Then, we easily can establish that

$$\underline{\hat{\mathbf{Q}}}^2 = \underline{\hat{\mathbf{Q}}}^{\dagger 2} = 0 \tag{III.28}$$

as well as

$$\{\underline{\hat{\mathbf{Q}}}, \underline{\hat{\mathbf{Q}}}^\dagger\} = \underline{\hat{\mathbf{Q}}}\,\underline{\hat{\mathbf{Q}}}^\dagger + \underline{\hat{\mathbf{Q}}}^\dagger\underline{\hat{\mathbf{Q}}} \tag{III.29}$$

$$= \underline{\hat{\mathbf{H}}} \tag{III.30}$$

where {,} denotes the anticommutator.

The eigenstates of $\underline{\hat{\mathbf{H}}}$ consist of vectors

$$\underline{\psi}_n = \begin{pmatrix} \psi_n^{(s,+)} \\ \psi_n^{(s,-)} \end{pmatrix} \tag{III.31}$$

and the supersymmetric Schrödinger equation reads

$$\underline{\hat{\mathbf{H}}}\underline{\psi}_n = E_n\underline{\psi}_n \tag{III.32}$$

The identity in eq III.32 results from the degeneracy of the spectra associated with $\hat{A}^{(s)}\hat{A}^{(s\dagger)}$ and $\hat{A}^{(s)\dagger}\hat{A}^{(s)}$. The eigenstates $|\psi_0^{(s,+)}\rangle$ are generally termed the boson sector, and the $|\psi_0^{(s,-)}\rangle$ are the fermion sector of the supersymmetric space in ψ_n. The charge operators transfer between sectors since

$$\underline{\hat{\mathbf{Q}}}^\dagger\begin{pmatrix} 0 \\ |\psi_n^{(s,-)}\rangle \end{pmatrix} = \begin{pmatrix} \hat{A}^{(s)\dagger}|\psi_n^{(s,-)}\rangle \\ 0 \end{pmatrix} \tag{III.33}$$

and

$$\underline{\hat{\mathbf{Q}}}\begin{pmatrix} |\psi_n^{(s,+)}\rangle \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ \hat{A}^{(s)}|\psi_n^{(s,+)}\rangle \end{pmatrix} \tag{III.34}$$

Of course, in this 1-D, nonrelativistic quantum case, the designations boson and fermion refer to the symmetry properties of the states rather than to different fundamental particles. As a final comment, we consider the action of $\hat{Q}$ and $\hat{Q}^\dagger$ on the ground state

$$\underline{\psi}_0 = \begin{pmatrix} |\psi_n^{(s,+)}\rangle \\ |\psi_n^{(s,-)}\rangle \end{pmatrix} \tag{III.35}$$

and

$$\underline{\hat{\mathbf{Q}}}\,\underline{\psi}_0 = \begin{pmatrix} 0 \\ 0 \end{pmatrix} = \underline{\hat{\mathbf{Q}}}^\dagger\underline{\psi}_0 \tag{III.36}$$

We conclude that the hindered rotor model is an example of good or unbroken SUSY.[10−12] These are systems for which the ground state of both the bosonic and fermionic sector has an energy of 0.

IV. Standard Quantum Mechanics of the Hindered Rotor

We now shall consider both a formal and computational study of the excited states of these new hindered rotor systems. We begin with considering a formally exact solution of the $\hat{H}_+$ Schrödinger equation. The solution for $\hat{H}_-$ can be obtained either by supersymmetry or by translation of φ by $\pm\pi$. The factored Schrödinger equation reads

$$\left[-\frac{d}{d\varphi} + \lambda\sin\varphi\right]\left[\frac{d}{d\varphi} + \lambda\sin\varphi\right]\psi_n^{(s,+)} = E_n\psi_n^{(s,+)} \tag{IV.1}$$

This is easily solved by integrating factors (or equivalently, by the Green's function), yielding

$$\psi_n^{(s,+)}(\varphi) = \psi_n^{(s,+)}(0)e^{\lambda(\cos\varphi - 1)} - E_n e^{\lambda\cos\varphi}\int_0^{\varphi}\int_0^{\varphi''}\psi_n^{(s,+)}(\varphi')e^{\lambda\cos\varphi' - 2\lambda\cos\varphi''}d\varphi' d\varphi'' \tag{IV.2}$$

We note that for $E_0 = 0$, we get our earlier result of

$$\psi_0^{(s,+)}(\varphi) = \psi_0^{(s,+)}(0)e^{\lambda\cos\varphi} \tag{IV.3}$$

It is also easily verified by substitution that eq IV.2 satisfies the Schrödinger eq IV.1. Of greatest interest are the excited states. In that case, we can see that eq IV.2 is an inhomogeneous, linear integral equation. Therefore, it does not lead to a familiar eigenvalue problem, and we expect there to be nontrivial solutions for all values of E. That is, by itself, eq IV.2 does not lead to quantization. Of course, the solution is to recall that the

TABLE 1: Energies for $\lambda = 1$ and 3

n	$\lambda = 1$	$\lambda = 3$
0	-8.22775×10^{-16}	-2.08273×10^{-13}
1	1.64737	5.39013
2	4.54059	9.39411
3	9.51758	13.9287
4	16.5098	20.7295

only allowed solutions must be periodic, with period 2π, and continuous

$$\psi_0^{(s,+)}(0) \equiv \psi_0^{(s,+)}(2\pi) \qquad \text{(IV.4)}$$

This condition immediately requires that

$$\int_0^{2\pi} \int_0^{\varphi''} \psi_n^{(s,+)}(\varphi') e^{\lambda \cos \varphi' - 2\lambda \cos \varphi''} d\varphi' d\varphi'' \equiv 0 \qquad \text{(IV.5)}$$

Therefore, eq IV.2 must be solved subject to the constraint of eq IV.5, and this is sufficient to produce quantization. This condition is the Bloch quantization condition, and the resulting quantum states are the band heads for a band structure.[14] The alternative approach is to solve by expanding in an appropriate basis. The most obvious choice is $e^{in\varphi}/(2\pi)^{1/2}$, $n = 0, \pm1, \pm2, ...$ since it is periodic on the domain in question, and these are

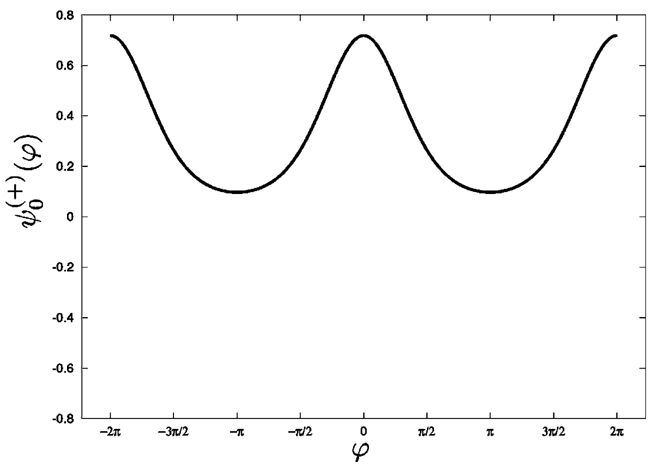

Figure 2. The exact and computed gound state is plotted versus φ; the results are visually indistinguishable.

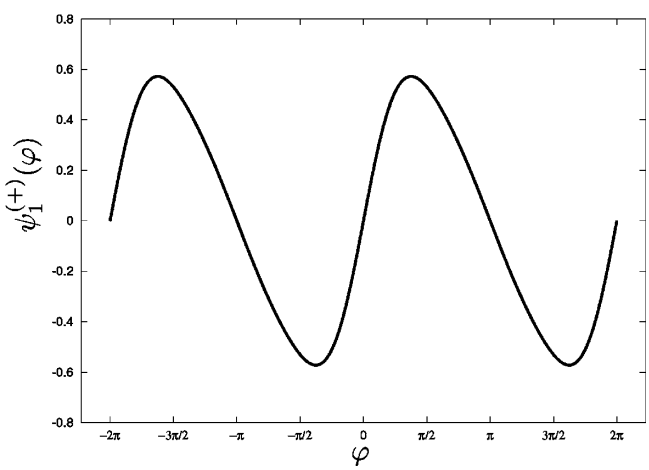

Figure 3. The state $\psi_1^{(+)}$ versus φ.

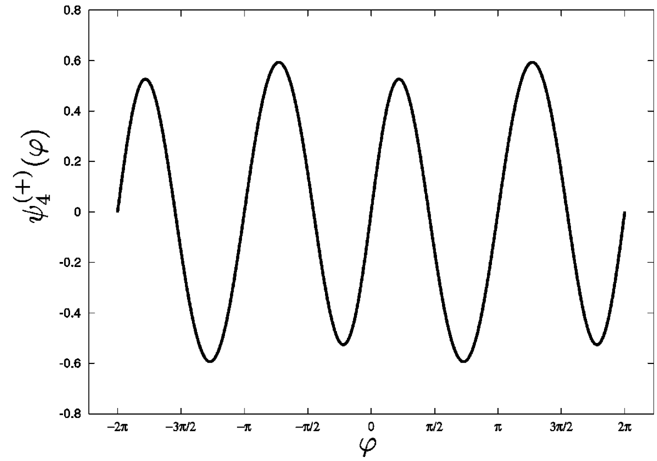

Figure 4. The state $\psi_4^{(+)}$ versus φ. Note the variation in the maxima and minima.

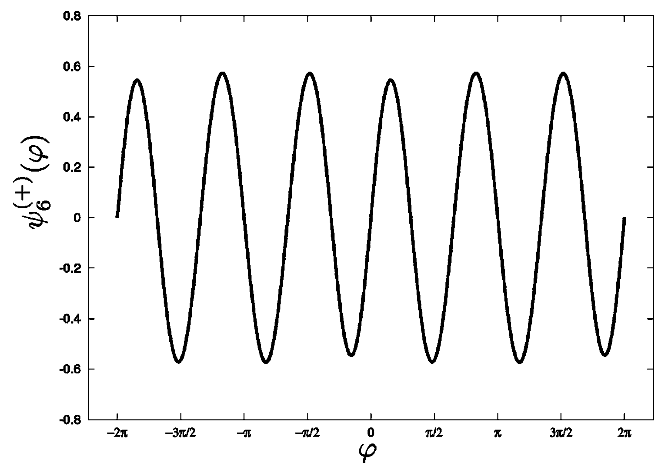

Figure 5. The state $\psi_6^{(+)}$ versus φ. The state resembles the $n = 3$ free rotor state, except for the variation in the maximum and minimum values.

also uncertainty minimizers of the periodic Heisenberg−Weyl algebra. The expansion is simple, and the Rayleigh−Ritz variational principle leads to[2]

$$\sum_{j=-N}^{N} \left[\left(j^2 + \frac{\lambda^2}{2} \right) \delta_{jj'} - \frac{\lambda^2}{4} \delta_{jj'-2} - \frac{\lambda^2}{4} \delta_{jj'+2} - \frac{\lambda}{2} \delta_{jj'-1} - \frac{\lambda}{2} \delta_{jj'+1} \right] C_j = E C_{j'} \qquad \text{(IV.6)}$$

This was solved numerically using LAPACK routines. The results for the energies are listed in Table 1 for $\lambda = 1$ and 3, $\langle \hat{s} \rangle = 0$, and $\langle \hat{k}_\varphi \rangle = 0$. The excited states are doubly degenerate and can be chosen to be purely real, with one set having even symmetry and the other odd symmetry. This is typical of SUSY quantum mechanics. The numerical and exact ground states are compared in Figure 2, where we note that convergence to the ground eigenstate to 10^{-6} was obtained with $j = 0, \pm1, \pm2, \pm3$ as the basis. The converged excited states are displayed in Figures 3−5. The accuracy of the results was tested using the Cauchy convergence criterion, with similar results to the ground state.

We see that the lower energy states are clearly modified relative to free rotor states. As one goes to higher energy states, they begin to appear like free rotor states. However, the effect of the hindering potential is seen in the fact that the maxima and minima are not uniform. As expected, this effect decreases as the energy increases.

V. Conclusions

We have found a periodic variant of the Heisenberg−Weyl algebra and shown that it leads to periodic raising and lowering operators. The $\Delta\hat{s}\Delta\hat{k}_\varphi$ minimum uncertainty state (with $\langle\hat{s}\rangle = \langle\hat{k}_\varphi\rangle = 0$) is annihilated by $\hat{A}^{(s)}$, and there are analogous operators arising from minimizing $\Delta\hat{c}\Delta\hat{k}_\varphi$. The minimum uncertainty depends on $\langle\hat{c}\rangle$. For values of $\langle\hat{c}\rangle$ close to 1, the minimum uncertainty state $\psi_0^{(s,+)}$ is a Gaussian in the neighborhood of $\varphi = 0$, but there is another state, $\psi_0^{(s,-)}$ that is also of minimum uncertainty and normalizable (due to the periodic nature of the states on the domain $[-\pi,\pi]$). In the more general situation, the periodic coherent states take the form

$$\psi_n^{(s)}(\varphi) = \psi_n^{(s)}(0)e^{\beta\cos\varphi + in\varphi} \tag{V.1}$$

where n plays the role of the dimensionless, angular momentum. Its expectation value is restricted to an integer due to the periodicity constraint.

The minimum $\Delta\hat{c}\Delta\hat{k}_\varphi$ uncertainty states (with $\langle\hat{s}\rangle = \langle\hat{k}_\varphi\rangle = 0$) can be chosen to be of the form $e^{i\alpha\sin\varphi}$. Furthermore, the product of the $\Delta\hat{c}$ and $\Delta\hat{s}$ uncertainty states also possesses the form of a general coherent Gaussian state in the $\varphi \approx 0$ neighborhood

$$e^{\beta^2(\cos\varphi - 1)}e^{i\alpha\sin\varphi} \approx e^{-\beta^2(\varphi^2/2)}e^{i\alpha\varphi} \tag{V.2}$$

where α is any real number.

In the remainder of the paper, where we analyze the resulting hindered rotor, we restricted $\langle\hat{s}\rangle = \langle\hat{k}_\varphi\rangle = 0$. This analysis could be repeated with general (but physically permitted) values of $\langle\hat{s}\rangle$, $\langle\hat{k}_\varphi\rangle$, and this may be of interest for later consideration.

We next showed that the operator $\hat{A}^{(s)}$ and its vacuum state, $e^{\beta(\cos\varphi - 1)}$ can be associated with a model describing hindered rotation. The Hamiltonian was obtained and shown to be an example of the supersymmetric form of quantum mechanics describing a hindered rotor. All of the relevant superoperators were explicitly constructed and shown to result in the usual boson and fermion sector description of the system.

Next, we considered the standard approach to this quantum system. The formal, exact solution for any energy E was presented, and quantization was shown to result from requiring periodicity and continuity of the allowed wave functions. We then carried out a variational numerical solution of the hindered rotor problem, obtaining the first nine states to a controlled accuracy in both the eigenvalue and the eigenstate.

There are a number of aspects that should be investigated further. First is a continued search for exact, analytical excited-state solutions to the hindered rotor, using the periodic Heisenberg−Weyl algebra, along with $\hat{A}^{(s)}$, $\hat{A}^{(s)\dagger}$. While our initial attempts have not been successful, we are hopeful that some generalization of the operator algebraic approach will prove successful.

Second, we are exploring the connection between the minimum uncertainty periodic Gaussians and constrained periodic minimum uncertainty states, that is, periodic minimum uncertainty μ-wavelets and closely related periodic Hermite distributed approximating functionals.[15,16] These are expected to be useful for quantum dynamics and other computations (e.g., the HDAFs have seen many such applications[17]). In addition, they should be useful for digital signal and image processing where periodicity of the filters is important.[18]

Finally, we anticipate that these hindered rotor states should prove useful as a basis set for treating perturbed hindered rotors. Such applications arise not only in chemical systems (e.g., internal rotation in organic systems) but also, for example, in surface physics.

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