Symmetries and solutions of the three-dimensional Paul trap

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1 Introduction

I first got to know of Joe (the speaker was MMN) because of his paper with Singh on the time-energy uncertainty relation [1]. [See the Appendix for this story.] To use the language of the discussions of this conference, the Eberly-Singh paper was “fundamental” though maybe not “useful.” But it certainly was fun. That is what we are presenting today. Something that is fun. We are going to discuss the Paul trap from a different point of view. We will discuss the Paul trap’s symmetries and use them to obtain the time-dependent solutions, without having to solve the mixed, second-order, partial, differential Schrödinger equation. We will be exemplifying something that Christopher Gerry alluded to yesterday: although the Heisenberg and Schrödinger formulations of quantum mechanics are equivalent, different things can be more transparent in one of them. It was Pauli who taught us this.

2 The Paul trap

The Paul trap provides a dynamically stable environment for charged particles [2]-[4] and has been widely used in fields from quantum optics to particle physics.

Paul gives a delightful mechanical analogy [4]. Think of a mechanical ball put at the center of a saddle surface. With no motion of the surface, it will fall off of the saddle. However, if the saddle surface is rotated with an appropriate frequency about the axis normal to the surface at the inflection point, the particle will be stably confined. The particle is oscillatory about the origin in both the \( x \) and \( y \) directions. But it’s oscillation in the \( z \) direction is restricted to be bounded from below by some \( z_0 > 0 \).

The potential energy can be parametrized as [2]

\[
V(x, y, z, t) = V_x(x, t) + V_y(y, t) + V_z(z, t),
\]

where

\[
V_x(x, t) = \frac{e}{2r_0^2} \mathcal{V}(t) x^2 \equiv g(t) x^2,
\]

\[
V_y(y, t) = \frac{e}{2r_0^2} \mathcal{V}(t) y^2 \equiv g(t) y^2,
\]

\[
V_z(z, t) = -\frac{e}{r_0} \mathcal{V}(t) z^2 \equiv g_3(t) z^2.
\]

These potentials can be used to set up the classical motion problem

\[
\ddot{x}_{cl} = F_x(x, t) = -\frac{dV_x(x, t)}{dx} = -2g(t)x_{cl},
\]

\[
\ddot{y}_{cl} = F_y(y, t) = -\frac{dV_y(y, t)}{dy} = -2g(t)y_{cl},
\]

\[
\ddot{z}_{cl} = F_z(z, t) = -\frac{dV_z(z, t)}{dz} = -2g_3(t)z_{cl}.
\]

The solutions to these equations are oscillatory Mathieu functions for the bound case [2]. The oscillatory motion is similar in the \( (x, y) \) directions but is different in the \( z \) direction, since \( g(t) \neq g_3(t) \).
3 The quantum-mechanical Paul trap

In the quantum mechanical treatment of the Paul trap, one must solve the Schrödinger equation, which in Cartesian coordinates has the form (\( \hbar = m = 1 \))

\[
S \Psi(x, y, z, t) = \{ \partial_{xx} + \partial_{yy} + \partial_{zz} + 2i \partial_t - 2g(t)(x^2 + y^2) - 2g_3(t)z^2 \} \Psi(x, y, z, t) = 0.
\] (8)

The time-dependent functions \( g \) and \( g_3 \) in Eq. (8) are

\[
g(t) = \frac{e}{2r_0^2} V(t), \quad g_3(t) = -\frac{e}{2r_0^2} V(t).
\] (9)

where

\[
V(t) = V_{\text{dc}} - V_{\text{ac}} \cos(\omega(t - t_0))
\] (10)

is the “dc” plus “ac time-dependent” electric potential that is applied between the ring and the end caps.

Exact solutions for the 1-dimensional, quantum case were first investigated in detail by Combescure [5]. In general, work has concentrated on the \( z \) coordinate, but not entirely [6]. Elsewhere [7], stimulated by the work of Ref. [8], we discussed the classical/quantum theory of the Paul trap in the \( z \)-direction.

The form of the Schrödinger equation (8) suggests that, in addition to the above Cartesian coordinate system, there is another natural coordinate system for this problem: the cylindrical coordinate system. Introducing such a change of variables,

\[
x = r \cos \theta, \quad y = r \sin \theta, \quad z = z,
\] (11)

the Schrödinger equation becomes

\[
S_{\text{cyl}} \Phi(r, \theta, z, t) = \left\{ \partial_{rr} + \frac{1}{r} \partial_r + \frac{1}{r^2} \partial_{\theta \theta} + \partial_{zz} + 2i \partial_t - 2g(t)r^2 - 2g_3(t)z^2 \right\} \Phi(r, \theta, z, t) = 0.
\] (12)

In addition, the forms of Eqs. (8) and (12) suggest that we can factorize the solutions and equations into the forms

\[
\Psi(x, y, z, t) = X(x, t)Y(y, t)Z(z, t),
\] (13)

\[
S_x X(x, t) = \{ \partial_{xx} + 2i \partial_t - 2g(t)x^2 \} X(x, t) = 0,
\] (14)

\[
S_y Y(y, t) = \{ \partial_{yy} + 2i \partial_t - 2g(t)y^2 \} Y(y, t) = 0,
\] (15)

\[
S_z Z(z, t) = \{ \partial_{zz} + 2i \partial_t - 2g_3(t)z^2 \} Z(z, t) = 0,
\] (16)

and

\[
\Phi(x, y, z, t) = \Omega(r, \theta, t)Z(z, t),
\] (17)

\[
S_{\text{cyl}} \Omega(r, \theta, t) = \left\{ \partial_{rr} + \frac{1}{r} \partial_r + \frac{1}{r^2} \partial_{\theta \theta} - 2g(t)r^2 \right\} \Omega(r, \theta, t) = 0.
\] (18)

Being physicists, we tend to blindly go ahead and accept this separation, ignoring the mathematical subtleties in separating coordinates in time-dependent partial differential equations. Fortunately, Rod insists on keeping me honest. But this procedure does turn out to be justified [9]. So, now we can just go blindly on.
4 Lie symmetries and separable coordinates

Lie symmetries for the Schrödinger equation (8) can be obtained by solving the operator equation [10, 11]

\[ [S, L] = \lambda(x, y, z, t)S. \] (19)

The operator \( S \) is one of the Schrödinger operators we have discussed, \( L \) is a generator of Lie symmetries, and \( \lambda \) is a function of the coordinates \( x, y, z, \) and \( t \). An operator \( L \) has the general form

\[ L = C_0 \partial_t + C_1 \partial_x + C_2 \partial_y + C_3 \partial_z + C, \] (20)

where the coefficient in each term is a function of the coordinates and time.

First we define what are going to be useful separable coordinates:

\[ x = \frac{x}{\phi^{1/2}(t)}, \quad y = \frac{y}{\phi^{1/2}(t)}, \quad z = \frac{z}{\phi^{1/2}_3(t)}, \quad t = t, \] (21)

and

\[ \rho = \sqrt{x^2 + y^2}, \quad \theta = \sin^{-1}\left( \frac{y}{\sqrt{x^2 + y^2}} \right), \quad z = \frac{z}{\phi^{1/2}_3(t)}, \quad t = t. \] (22)

The \( t \)-dependent functions \( \phi(t) \) and \( \phi_3(t) \) are given by

\[ \phi = 2\xi\bar{\xi}, \quad \phi_3 = 2\xi_3\bar{\xi}_3, \] (23)

where \{\( \xi(t), \bar{\xi}(t) \)\} and \{\( \xi_3(t), \bar{\xi}_3(t) \)\} are the complex solutions of the second-order, linear, differential equations in time

\[ \ddot{\gamma} + 2g(t)\gamma = 0, \quad \ddot{\gamma}_3 + 2g_3(t)\gamma_3 = 0, \] (24)

respectively, and satisfy the Wronskians

\[ W(\xi, \bar{\xi}) = W(\xi_3, \bar{\xi}_3) = -i. \] (25)

Equations (24) are the same as the classical equations of motion (5)-(7) for the Paul trap. The solutions are the same Mathieu functions. For certain values of the parameters in the potential (1), the solutions are bound, meaning the charged particle is indeed “trapped” [2]. This shows a connection between classical and quantum dynamics.

5 Cartesian symmetries

For this exercise we can concentrate only on the \( z \) coordinate, since formally the results are the same for the \( x \) and \( y \) solutions, with the exception that the \( \xi_3 \)'s and \( g_3 \)'s, etc., lose the subscripts 3. [Elsewhere, we will discuss the symmetries of the Paul trap in much greater detail [9].]

One can find, or simply verify, that the Schrödinger equation has the symmetry operators

\[ J_{z-} = \xi_3 \partial_z - i\bar{\xi}_3z = +\frac{1}{\sqrt{2}} \left( \frac{\bar{\xi}_3}{\xi_3} \right)^{\frac{1}{2}} \left[ \partial_z + z \left( 1 - \frac{i}{2} \dot{\phi}_3 \right) \right], \] (26)

\[ J_{z+} = -\bar{\xi}_3 \partial_z + i\xi_3z = -\frac{1}{\sqrt{2}} \left( \frac{\xi_3}{\bar{\xi}_3} \right)^{\frac{1}{2}} \left[ \partial_z - z \left( 1 + \frac{i}{2} \dot{\phi}_3 \right) \right]. \] (27)

These operators satisfy the nonzero commutation relation

\[ [J_{z-}, J_{z+}] = I, \] (28)
and so form a complex Heisenberg Weyl algebra $w^c$. This means that the operators

generate a set of “number states” given by

$$J_z Z_{nz}(z, t) = \sqrt{n_z} Z_{nz-1}(z, t), \quad (29)$$

$$J_{z+} Z_{nz}(z, t) = \sqrt{n_z + 1} Z_{nz+1}. \quad (30)$$

There is also an $su(1, 1)$ algebra, which we will not go into here. This is a generalization of the “squeeze algebra.”

A word of caution. The states $Z_{nz}(z, t)$ are not to be construed as energy eigenstates. $Z_{nz}$ is a solution to the time-dependent Schrödinger equation (16). It is generally not an eigenfunction of the Hamiltonian. That is,

$$i \partial_t Z_{nz} = H Z_{nz} = i \left[ i \partial_t Z_{nz} \over Z_{nz} \right] Z_{nz} \neq |\text{Const}| Z_{nz}. \quad (31)$$

So, to keep John Klauder from getting mad at me, we use the terminology “extremal state” for $Z_0$ and “higher-order” states for $Z_{nz}$. We restrict the terms “ground state” and “excited state” for problems which allow eigenstates of the Hamiltonian.

Eq. (29) is a simple first order differential equation for $Z_0$:

$$J_z - Z_0(z, t) = 0. \quad (32)$$

Solving it yields

$$Z_0(z, t) = f(t) \exp \left\{ -z^2 \left[ 1 - i \dot{\phi}_3 \over \sqrt{2} \right] \right\}, \quad (33)$$

where the proportionality constant, $f$ must be a function of $t$.

A first idea might be to take this proportionality constant as the “normalization constant,” $[\pi \dot{\phi}_3(t)]^{-1/4}$. This would conserve the probability, as one would want for the time-development of a unitary Hamiltonian. But this turns out to be incorrect. Such a solution does not satisfy the Schrödinger equation (16). Indeed, putting Eq. (33) into Eq. (16) yields a first order differential equation in $t$ for $f(t)$. The resulting normalized extremal-state solution is

$$Z_0(z, t) = (\pi \dot{\phi}_3)^{-1/4} \left( \xi_3 \over \xi_3 \right)^{\frac{\dot{\phi}_3}{2}} \exp \left\{ -z^2 \left[ 1 - i \dot{\phi}_3 \over \sqrt{2} \right] \right\} \exp \left\{ -{z^2 \over 2} \left[ 1 - i \dot{\phi}_3 \over 2 \right] \right\}. \quad (34)$$

So why is the phase factor $(\xi_3/\xi_3)^{1/4}$ there? It is there because, in this time-dependent Schrödinger equation, it is the necessary generalization of the simple-harmonic oscillator ground-state energy exponential, $\exp[-i\hbar \omega/2]$. (This follows since $\xi_3(t) \rightarrow (2\omega)^{-1/2} \exp[i\omega t]$.) This phase factor is necessary [12, 13, 14] for Eq. (34) to be a solution of Eq. (16).

Now repeated application of Eq. (30) gives

$$Z_{nz}(z, t) = [n_z!]^{-1/2} [J_{z+}]^{n_z} Z_0(z, t). \quad (35)$$

But the right hand side of Eq. (35) is proportional to [9] the Rodrigues formula for the Hermite polynomials [15]. Using this yields the result

$$Z_{nz}(z, t) = (2^{n_z} n_z!)^{-1/2} (\pi \dot{\phi}_3)^{-1/4} \left( \xi_3 \over \xi_3 \right)^{\frac{\dot{\phi}_3}{2}} (n_z + \frac{1}{2}) \quad H_{nz}(z) \exp \left\{ -z^2 \left[ 1 - i \dot{\phi}_3 \over 2 \right] \right\} . \quad (36)$$
The forms of \( X_{n_x}(x,t) \) and \( Y_{n_y}(y,t) \) follow immediately by just changing notation,

\[
X_{n_x}(x,t) = Z_{n_z-n_x}(z \to x, \xi_3 \to \xi, \phi_3 \to \phi, t),
\]

\[
Y_{n_y}(y,t) = Z_{n_z-n_y}(z \to y, \xi_3 \to \xi, \phi_3 \to \phi, t),
\]

so that

\[
\Psi_{n_z,n_y,n_x}(x,y,z,t) = X_{n_x}(x,t)Y_{n_y}(y,t)Z_{n_z}(z,t).
\]

### 6 Polar symmetries

In what is intuitively interesting, finding the symmetries for the polar coordinates amounts to considering complex linear combinations of the Cartesian operators. Take the following two pairs of operators which form the basis of two Heisenberg-Weyl algebras [11]:

\[
a_- = a_+^\dagger = \sqrt{\frac{1}{2}}(J_{x-} + iJ_{y-}) = \sqrt{\frac{1}{2}} \left[ \xi(\partial_x + i\partial_y) - i\dot{\xi}(x + iy) \right],
\]

\[
= \frac{1}{2} \left( \frac{\xi}{\xi} \right)^{1/2} e^{i\theta} \left[ \partial_\rho + \frac{i}{\rho} \partial_\theta + \rho \left( 1 - \frac{i}{2} \dot{\phi} \right) \right],
\]

\[
c_- = c_+^\dagger = \sqrt{\frac{1}{2}}(J_{x-} - iJ_{y-}) = \sqrt{\frac{1}{2}} \left[ \xi(\partial_x - i\partial_y) - i\dot{\xi}(x - iy) \right],
\]

\[
= \frac{1}{2} \left( \frac{\xi}{\xi} \right)^{1/2} e^{-i\theta} \left[ \partial_\rho - \frac{i}{\rho} \partial_\theta + \rho \left( 1 - \frac{i}{2} \dot{\phi} \right) \right].
\]

If we add to the above four operators \( I \), the operator

\[
K = J_{x+}J_{x-} + J_{y+}J_{y-} + 1 = a_+a_- + c_+c_- + 1,
\]

and the angular momentum operator

\[
L_z = i(y\partial_x - x\partial_y) = -i\partial_\theta,
\]

we have that the set \( \{ I, a_\pm, c_\pm, K, L_z \} \) forms a closed algebra. Further, if we make the transformations

\[
f \equiv \frac{1}{2} (K - L_z) = a_+a_- + \frac{1}{2}, \quad (44)
\]

\[
d \equiv \frac{1}{2} (K + L_z) = c_+c_- + \frac{1}{2}, \quad (45)
\]

we see that the symmetry algebra has two oscillator subalgebras, \( \{ f, a_\pm, I \} \) and \( \{ d, c_\pm, I \} \), which have only the identity operator, \( I \), in common. Therefore, the algebra is \( G_{x,y} = so_8(1) + so_1(1) \), with the two Casimir operators \( C_1 = a_+a_- - f = -\frac{3}{2} \) and \( C_2 = c_+c_- - d = -\frac{3}{2} \).

We restrict ourselves to the representations of \( os(1) \) that are bounded below; namely, \( \uparrow_{-1/2} \to \uparrow_{-1/2} \). Let \( \Omega_{n,m} \) be a member of the set of common eigenfunctions of \( f \) and \( d \) spanning the representation space. Then, for \( (n, m) \in \mathbb{Z}_0^+ \), we have

\[
f\Omega_{n,m} = \left( n + \frac{1}{2} \right) \Omega_{n,m}, \quad d\Omega_{n,m} = \left( m + \frac{1}{2} \right) \Omega_{n,m}, \quad (46)
\]

\[
a_-\Omega_{n,m} = \sqrt{n+1}\Omega_{n-1,m}, \quad c_-\Omega_{n,m} = \sqrt{m}\Omega_{n,m-1}, \quad (47)
\]

\[
a_+\Omega_{n,m} = \sqrt{n+1}\Omega_{n+1,m}, \quad c_+\Omega_{n,m} = \sqrt{m+1}\Omega_{n,m+1}, \quad (48)
\]

\[
L_z\Omega_{n,m} = (f - d)\Omega_{n,m} = (m - n)\Omega_{n,m}, \quad (49)
\]

\[
K\Omega_{n,m} = (d + f)\Omega_{n,m} = (n + m + 1)\Omega_{n,m}, \quad (50)
\]
In order that the spectrum of $d$ and $f$ be bounded below, we also have
\[ a_- \Omega_{0,0} = 0, \quad c_- \Omega_{0,0} = 0. \] (51)

Eqs. (43) and (49) immediately tell us that the (normalized) $\theta$ dependence of the $\Omega_{n,m}(r, \theta, t)$ can be given by
\[ \Omega_{n,m}(r, \theta, t) = R_{n,m}(r, t) \Theta_{n,m}(\theta) = R_{n,m}(r, t) \frac{\exp[i(m-n)\theta]}{\sqrt{2\pi}}. \] (52)

Therefore, $\Omega_{0,0}(r, \theta, t)$ is a function only of $r$ or $\rho$ and $t$. In this $(n, m) = (0, 0)$ case, both the equations in (51) have the same first-order differential form. So, we can solve for $\Omega_{0,0}$ similarly to as was done for the $Z_0$ solution. The normalized solution to the Schrödinger equation (18) is found to be
\[ \Omega_{0,0}(r, \theta, t) = \frac{1}{\sqrt{2\pi}} \left[ \frac{2}{\theta} \right]^{1/2} \left( \frac{\xi^2}{\lambda^2} \right)^{1/2} \exp \left\{- \rho^2 \left[ 1 - \frac{i}{2} \right] \right\} = X_0(x, t) Y_0(y, t). \] (53)

Repeated application of Eqs. (48) gives us the general result:
\[ \Omega_{n,m}(\rho, \theta, t) = (n!m!)^{-1/2} a_n^m \omega_{\rho, \theta, t}. \] (54)

This turns out also to be a Rodrigues-type formula, although more complicated than before [9]. This time it is for the generalized Laguerre polynomials [15]. The end result turns out to be
\[ \Omega_{n,m}(r, \theta, t) = \exp[i(m-n)\theta] \frac{(-)^k k!}{n!m!} \left( \frac{2}{\phi(t)} \right)^{1/2} \left( \frac{\xi^2}{\lambda^2} \right)^{1/2} \rho^{n-m} \nu_k^{(n-m)}(\rho^2) \exp \left\{- \rho^2 \left[ 1 - \frac{i}{2} \right] \right\}, \] (55)
\[ k \equiv \frac{1}{2}(n + m - |m - n|). \] (56)

Now let us change to the more standard cylindrical quantum numbers:
\[ \ell = |\ell_z|, \quad \ell_z = m - n, \quad n_r = m + n \geq 0. \] (57)

We find that
\[ \Omega_{n,m}(r, \ell) \rightarrow R_{n,r,\ell}(r, \theta) \Theta_{\ell_z}(\theta), \] (58)
\[ \Theta_{\ell_z}(\theta) = \frac{\exp[i \ell_z \theta]}{\sqrt{2\pi}}, \] (59)
\[ R_{n,r,\ell}(r, \ell) = (-1)^{(n-r)/2} \left[ \frac{2}{\phi(t)} \left[ \frac{n_r - \ell}{n_r + \ell} \right] \left( \frac{\xi^2}{\lambda^2} \right)^{1/2} \right] \rho^{n_r-\ell} \bar{\nu}_{\ell_z}^{(n_r-\ell)}(\rho^2) \exp \left\{- \rho^2 \left[ 1 - \frac{i}{2} \right] \right\}. \] (60)

Except for our minus-sign phase convention, Eq. (60) resembles the standard result for the ordinary two-dimensional harmonic oscillator [16].

This standard solution has the known property that $n_r$ and $\ell_z$ cannot differ by an odd integer to allow a normalizable solution. \[ \frac{1}{2}(n_r - \ell) \] must be an integer. If one
solves the Schrödinger equation directly, this falls out, but the physical reason is not transparent. However, from the symmetry point of view, the reason is clear. The $n$ and $m$ quantum numbers, which reflect the fundamental symmetries, can be all non-negative integers. The $n_r$ and $\ell_z$ quantum numbers reflect a rotation of the axes by $45^\circ$. (See figure 1.) So, reaching the allowed positions of quantum numbers along these diagonals, scaled by $1/\sqrt{2}$, means all integer values of $(n_r, \ell_z)$ are not allowed.

Fig. 1. A plot of the allowed quantum numbers for the polar coordinates of the Paul trap. Shown are the $(n, m)$ quantum numbers of Eqs. (54) and (55) as well as the $(n_r, \ell_z)$ quantum numbers of Eqs. (57) and (60).

This is similar in spirit to Pauli’s being able to show, by symmetry methods, that there is an extra conserved quantity, the Runge-Lenz vector, on the hydrogen atom. This allowed an understanding of the extra degenerate quantum number.

Finally, we can write out the complete solution in spherical coordinates as

$$\Phi_{n_r, \ell_z, n_z}(x, y, z, t) = R_{n_r, \ell}(r, t)\Theta_{\ell_z}(\theta)Z_{n_z}(z, t).$$

(61)

Appendix: Getting to know (about) Joe

Peter Carruthers, who was my advisor at Cornell, had a great ability to find talent in physicists. He also was very perceptive about the qualities of people, being a well-known lover of life. For reasons that will become clear below, let me give you two examples of Pete’s first ability.
i) We graduate students were amused by this new, young, hot-shot, assistant professor who was going to publish a famous paper. We were more amused when he made associate professor. Later, I heard of the move to make him full professor. (From lack of being there some of these details must be off.) It was boiling down to Hans Bethe’s call. Pete figuratively pounded Hans’ desk top telling Bethe he had to promote this guy. In the end the youngster got his full professorship, published his paper (on the renormalization group), and the rest is the history of Ken Wilson.

ii) When Pete became division leader at Los Alamos, Pete decided to hire as a staff member a young guy who had had an unproductive postdoc career – solely on the basis that Pete sensed creativity. Pete had to hide him in the Division Office, not a group, because funding could not be justified. He just sat around the corner, playing with his HP calculator, getting funny numbers again and again, leading to the period-doubling, chaos revolution of Mitchell Feigenbaum.

I mention this all in the context of when I first heard of Joe Eberly. (It was not when I was at Cornell, because then my main contact with Rochester was with the wild man of the time, Robert Marshak.) It was when Pete came out to Los Alamos. I asked him if he had seen the new paper by Eberly and Singh [1] on the time-energy uncertainty relation that had referred to our work. Pete said he had, and had liked it. Then he remarked that Eberly “is very smart.” Being properly impressed, I figuratively wrote down Joe’s name in my black book of smart guys. Then Pete said he’s also a nice a guy. So, Joe also went into the “nice guy” book. Most of us, if we are honest, must admit to really wanting to be in the first book. But Joe is in both books, and that is why we are all here today to honor him.

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