Time dependence of variables in the quantum-mechanical and classical Coulomb problems, and the dynamical algebra so(4,2)

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Hermitian tilted so(4,2) operators are constructed, acting on the bound states of the Coulomb problem, and are shown to have simple time dependence in the Heisenberg picture. The periodic time dependence of the corresponding classical variables can be regarded as a consequence of their simple geometrical interpretation and their simple expressions in terms of action-angle variables. Corresponding results are indicated for unbound states.

INTRODUCTION

The Coulomb problem with Hamiltonian

$$
H = \frac{1}{2}p^2 - r^{-1}
$$
 (1)

(here $p = |p|$, $r = |r|$, $\hbar = m = e = 1$), is one of the best known and most important problems in quantum mechanics. In particular, the solution of the eigenvalue problem^{1,2} for \hat{H} and the determination of the Coulomb Green's function³ have been known for a long time. More recently, several authors have discussed related quasicoherent states and their time evolution in the Schrödinger picture. 4 On the other hand, although it is often remarked that the relationship between a quantum system and its classical counterpart is brought out most clearly by working in the Heisenberg picture for the former, and although the classical Kepler-Coulomb problem is exactly soluble, the time dependence does not seem to have been explicitly determined for any nonconstant observable of the quantum Coulomb system, treated in the Heisenberg picture, Indeed, Heisenberg's equations of motion have been solved explicitly for only a few of the "exactly soluble" problems of quantum mechanics.⁵

A complete set of commuting constants for the Coulomb system is given by H , L·L, and L_3 , where $L = r \times p$; the time dependence of other observables is determined formally by, for example,

$$
\mathbf{r}(t) = e^{iHt}\mathbf{r}(0)e^{-iHt} \t{,} \t(2)
$$

but such formulas give no immediate information about the nature of the time dependence particular to the Coulomb problem.

Heisenberg's equations for r and p take the same form as Hamilton's equations for the classical system,

$$
\dot{\mathbf{r}} = \mathbf{p}, \quad \dot{\mathbf{p}} = -\frac{\mathbf{r}}{r^3} \tag{3}
$$

and even classically these cannot be solved to get the time dependence of r and p explicitly. However, in the classical case other canonically conjugate sets of variables whose time dependence can be found, in particular, action-angle variables,⁶ can be defined in terms of r and p, and one may ask to what extent this is possible in the quantum case.

OUANTUM AND CLASSICAL so(4,2) VARIABLES

It is known⁷ that the linear span $\mathcal V$ of the (bound state) eigenvectors of H carries a representation of the Lie algebra so(4,2), which can be used to calculate and characterize the discrete spectrum. $8-10$ The basis operators of an equivalent representation, more convenient for calculations, are given by L and (in the notation of Ref. 11)

$$
\Gamma_0 = \frac{1}{2}(rp^2 + r), \quad \Gamma_4 = \frac{1}{2}(rp^2 - r), \nT = r \cdot p - i, \quad \Gamma = rp, \nA = \frac{1}{2}(rp^2 - r) - (r \cdot p - i)p, \nM = \frac{1}{2}(rp^2 + r) - (r \cdot p - i)p.
$$
\n(4)

The Hamiltonian H is not in this Lie algebra, but a similarity transformation K exists, the so-called "tilt,"^{8,9} which carries Γ_0 into

$$
\Gamma_0^* = K^{-1} \Gamma_0 K = (-2H)^{-1/2} , \qquad (5)
$$

thus relating the discrete spectrum of H to that of Γ_0 and Γ_0^* . The eigenvalue of Γ_0^* is then n, the "principal quan- Γ_0^* . The eigenvalue of Γ_0^* is then *n*, the "principal quantum number," and accordingly we sometimes write *N* in place of Γ_0^* in what follows. On an eigenvector ϕ_n of *H* place of Γ_0^* in what follows. On an eigenvector ϕ_n of H with eigenvalue $(-1/2n^2)$, the tilt is given by

$$
K = \alpha(n) \exp[iT \ln(n)] \tag{6}
$$

(where α is a function to be determined), and can be regarded as an energy-dependent scale transformation.^{8,9} On \mathcal{V} , K is therefore given by

$$
K = \left[\sum_{k=0}^{\infty} (iT)^{k} [\ln(N)]^{k} / k! \right] \alpha(N)
$$

= exp[iT:ln(N)]\alpha(N) , \t(7)

where the colon indicates the ordering: powers of T to the left of powers of $ln(N)$.

We now define tilted $so(4,2)$ operators Γ_0^* , $\Gamma_4^* = K^{-1} \Gamma_4 K$, etc. To calculate the forms of these operators on V , we note firstly from (6) that K^{-1} on any eigenvector of Γ_0 with eigenvalue *n* must be given by $exp[-iT \ln(n)]/\alpha(n)$, since $K\phi_n$ is a typical such eigenvector. Then, for example, since $(\Gamma_4 + iT)$ shifts the value of Γ_0 up by one unit, we have

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$$
(\Gamma_{4}^{*} + iT^{*})\phi_{n} = \exp[-iT \ln(n+1)][\frac{1}{2}(\Gamma_{4} + \Gamma_{0}) + \frac{1}{2}(\Gamma_{4} - \Gamma_{0}) + iT]\exp[iT \ln(n)]\beta(n)\phi_{n}
$$

\n
$$
= \{\frac{1}{2}(\Gamma_{4} + \Gamma_{0})\exp[-i(T+i)\ln(n+1) + iT \ln(n)]
$$

\n
$$
+ \frac{1}{2}(\Gamma_{4} - \Gamma_{0})\exp[-i(T-i)\ln(n+1) + iT \ln(n)]
$$

\n
$$
+ iT \exp[-iT \ln(n+1) + iT \ln(n)]\beta(n)\phi_{n}
$$

\n
$$
= [\frac{1}{2}(\Gamma_{4} + \Gamma_{0})(n+1) + \frac{1}{2}(\Gamma_{4} - \Gamma_{0})(n+1)^{-1} + iT]\exp[iT \ln[n/(n+1)]]\beta(n)\phi_{n}, \qquad (8)
$$

where ${\beta(n) = \alpha(n)/\alpha(n + 1)}$. Here we have exploited also the $so(4, 2)$ commutation relations between T and $(\Gamma_4 \pm \Gamma_0)$. It follows from (8) that on \mathcal{V} ,

$$
\Gamma_4^* + iT^* = \frac{1}{2}rp^2F(N+1) - \frac{1}{2}rF(N+1)^{-1} + i(\mathbf{r} \cdot \mathbf{p} - i)F,
$$

$$
F = \exp\{i(\mathbf{r} \cdot \mathbf{p} - i) \cdot \ln[N(N+1)^{-1}]\}\beta(N) \qquad (9)
$$

using the same ordering notation as in (7).

Proceeding in this way we find that 12 in addition to (5) and (9) ,

$$
\mathbf{L}^* = \mathbf{L} = \mathbf{r} \times \mathbf{p}, \quad \mathbf{A}^* = \frac{1}{2} \left[\mathbf{p} \times \mathbf{L} - \mathbf{L} \times \mathbf{p} - 2\frac{\mathbf{r}}{r} \right] N ,
$$
\n
$$
\mathbf{\Gamma}^* + i \mathbf{M}^* = r \mathbf{p} \mathbf{F} + i \left[\frac{1}{2} \mathbf{r} \mathbf{p}^2 - (\mathbf{r} \cdot \mathbf{p} - i) \mathbf{p} \right] \mathbf{F} (N+1)
$$
\n
$$
+ \frac{1}{2} i \mathbf{r} \mathbf{F} (N+1)^{-1} ,
$$
\n
$$
\mathbf{\Gamma}^* - i \mathbf{T}^* = \frac{1}{2} r \mathbf{p}^2 G (N-1) - \frac{1}{2} r G (N-1)^{-1} - i (\mathbf{r} \cdot \mathbf{p} - i) G ,
$$
\n
$$
\mathbf{\Gamma}^* - i \mathbf{M}^* = r \mathbf{p} G - i \left[\frac{1}{2} \mathbf{r} \mathbf{p}^2 - (\mathbf{r} \cdot \mathbf{p} - i) \mathbf{p} \right] G (N-1)
$$
\n
$$
- \frac{1}{2} i \mathbf{r} G (N-1)^{-1} ,
$$
\n
$$
G = \exp\{i (\mathbf{r} \cdot \mathbf{p} - i) : \ln[N(N-1)^{-1}]\} [\beta(N-1)]^{-1} .
$$
\n(10)

These expressions are consistent with general forms for so(4, 1) operators in the Coulomb problem obtained by Musto¹³ and by Pratt and Jordan,¹⁴ who did not, howev er, consider the question of time dependence.

The choice $\alpha(N) = N$, so that $\beta(N) = N(N + 1)^{-1}$, makes the tilted $so(4,2)$ operators (5) , (9) , and (10) Hermitian, as can be checked by evaluating their matrix elements in the coordinate representation. They satisfy the same commutation relations amongst themselves as the untilted operators although they are much more complicated functions of the variables r and p. However, in contrast to the untilted operators, they do have simple time dependence, determined by equations like (2), because they all have simple commutators with Γ_0^* , which is related to the Hamiltonian by (5) . In particular, L^* , and Γ_0^* itself, are constants of the motion, as is A^* , which is, apart from the factor N , the Runge-Lenz-Pauli vector.² The nonconstant operators can be resolved into shift operators for N and we have, e.g.,

$$
\Gamma_4^*(t) + iT^*(t)
$$

= exp(- $\frac{1}{2}$ itN⁻²)[$\Gamma_4^*(0) + iT^*(0)$]exp($\frac{1}{2}$ itN⁻²)
= [$\Gamma_4^*(0) + iT^*(0)$]exp($\frac{1}{2}$ itN⁻² - $\frac{1}{2}$ it (N + 1)⁻²]
= [$\Gamma_4^*(0) + iT^*(0)$]exp[it (N + $\frac{1}{2}$)N⁻²(N + 1)⁻²],

and in a similar way we find

$$
\Gamma^*(t) + i\mathbf{M}^*(t)
$$

\n= $[\Gamma^*(0) + iM^*(0)] \exp[i t (N + \frac{1}{2})N^{-2}(N + 1)^{-2}]$,
\n
$$
\Gamma^*_4(t) - iT^*(t)
$$

\n= $\exp[-it (N + \frac{1}{2})N^{-2}(N + 1)^{-2}][\Gamma^*_4(0) - iT^*(0)]$,
\n
$$
\Gamma^*(t) - i\mathbf{M}^*(t)
$$

\n= $\exp[-it (N + \frac{1}{2})N^{-2}(N + 1)^{-2}][\Gamma^*(0) - i\mathbf{M}^*(0)]$. (12)

While the difference between the first and last lines of (11) , for example, may seem slight, it is only the latter form which directly reflects the nature of time dependence peculiar to the Coulomb problem. In order to appreciate this more fully, it is necessary to compare {5),(9), (10), (11), and (12) with the corresponding classical formulas. These can be obtained by first introducing explicitly \hbar , m, and e (replacing r by r/a , p by pa/ \hbar , H by H/E , N by $NE^{1/2}$, and t by tE/ \hbar , where $a = \hbar^2$ /me² and $E = me^4/\hbar^2$, then multiplying each so(4,2) operator by \hbar to give it dimensions of angular momentum, and finally letting \hbar go formally to 0. For example, (9) becomes, in dimensional form,

$$
\Gamma_4^* + iT^* = \frac{1}{2}rp^2F[\bar{N} + (\hbar/me^2)] - \frac{1}{2}rF[\bar{N} + (\hbar/me^2)]^{-1} + i(r \cdot \mathbf{p} - i\hbar)F,
$$

$$
\bar{N} = (-2mH)^{-1/2}, \quad F = \exp\{- (i/\hbar)(\mathbf{r} \cdot \mathbf{p} - i\hbar) : \ln[1 + (\hbar/me^2)\bar{N}^{-1}]\} \bar{N}[\bar{N} + (\hbar/me^2)]^{-1}
$$
(13)

and goes in the classical limit to

$$
\Gamma_4^* + iT^* = \frac{1}{2} [rp^2 \overline{N} - (r/\overline{N}) + 2i\mathbf{r} \cdot \mathbf{p}] U ,
$$

$$
U = \exp(-i\mathbf{r} \cdot \mathbf{p}/me^2 \overline{N}) . \qquad (14)
$$

Similarly (11) goes to

$$
\Gamma_4^*(t) + iT^*(t) = [\Gamma_4^*(0) + iT^*(0)] \exp(it/V) ,
$$

$$
V = m^2 e^2 \overline{N}^3 \ . \qquad (15)
$$

 (11)

Altogether, we find in the limit

$$
\Gamma_0^* = me^2 \overline{N}, \quad \mathbf{L}^* = \mathbf{L} = \mathbf{r} \times \mathbf{p} ,
$$
\n
$$
\mathbf{A}^* = [\mathbf{p} \times \mathbf{L} - me^2(\mathbf{r}/r)] \overline{N} ,
$$
\n
$$
\Gamma_4^* \pm iT^* = \frac{1}{2} [rp^2 \overline{N} - (r/\overline{N}) \pm 2ir \cdot \mathbf{p}] U^{\pm 1} ,
$$
\n
$$
\Gamma^* \pm i \mathbf{M}^* = [rp \pm \frac{1}{2}i (rp^2 - 2(r \cdot \mathbf{p}) \mathbf{p}) \overline{N} \pm \frac{1}{2}i (r/\overline{N})] U^{\pm 1} ,
$$
\n(16)

with Γ_0^* , L^* , and A^* constant, and with

$$
\Gamma_4^*(t)\pm iT^*(t) = [\Gamma_4^*(0)\pm iT^*(0)]\exp(\pm it/V) ,
$$

\n
$$
\Gamma^*(t)\pm i\mathbf{M}^*(t) = [\Gamma^*(0)\pm i\mathbf{M}^*(0)]\exp(\pm it/V) .
$$
 (17)

These classical tilted so(4,2) variables are equivalent to ones obtained in the context of the classical problem by Györgyi. However, he did not explicitly derive the time dependence of the corresponding quantum-mechanical observables. The classical variables can be expressed simply, in a way that clarifies the nature of their time dependence, in terms of the classical action-angle variables⁶

$$
J_1 = L_3^*, \quad J_2 = | L^* |, \quad J_3 = me^2 \overline{N} ,
$$

\n
$$
\omega_1 = \phi + \arctan[J_1 \cos\theta/(J_2^2 \sin^2\theta - J_1^2)^{1/2}],
$$

\n
$$
\omega_2 = -\arccos\{(J_2^2 - me^2r)J_3/[me^2r(J_3^2 - J_2^2)^{1/2}]\},
$$

\n
$$
-\arctan[J_2 \cos\theta/(J_2^2 \sin^2\theta - J_1^2)^{1/2}],
$$

\n
$$
\omega_3 = \arccos\{(J_3^2 - me^2r)/[J_3(J_3^2 - J_2^2)^{1/2}]\} - [2me^2r/J_3^2 - m^2e^4r^2/J_3^4 - J_2^2/J_3^2]^{1/2},
$$

where θ and ϕ are the polar angles of r. Since $H = -\frac{1}{2}me^4/J_3^2$, it follows that not only the actions but also ω_1 and ω_2 are constants, and also that ω_3 satisfies

$$
\dot{\omega}_3 = me^4/J_3^3 = 1/V = \text{const} \tag{19}
$$

We find that the classical tilted so(4,2) variables can be expressed (with $L^*_{\pm} = L^*_{1} \pm iL^*_{2}$, etc.) as

$$
\Gamma_0^* = J_3, \quad L_3^* = J_1, \quad L_{\pm}^* = \pm i (J_2^2 - J_1^2)^{1/2} \exp(\pm i\omega_1),
$$
\n
$$
A_3^* = -(J_2^2 - J_1^2)^{1/2} (J_3^2 - J_2^2)^{1/2} (\sin\omega_2) / J_2,
$$
\n
$$
A_{\pm}^* = (J_3^2 - J_2^2)^{1/2} (\cos\omega_2 \pm iJ_1 \sin\omega_2 / J_2) \exp(\pm i\omega_1),
$$
\n
$$
\Gamma_4^* \pm iT^* = (J_3^2 - J_2^2)^{1/2} \exp(\pm i\omega_3),
$$
\n
$$
\Gamma_3^* \pm iM_3^* = -(J_2^2 - J_1^2)^{1/2} (\cos\omega_2 \pm iJ_3 \sin\omega_2 / J_2)
$$
\n
$$
\times \exp(\pm i\omega_3),
$$
\n
$$
\Gamma_{\pm}^* + iM_{\pm}^* = [-(J_2 \pm J_1 J_3 / J_2) \sin\omega_2 + i (J_3 \pm J_1) \cos\omega_2]
$$
\n
$$
\times \exp[i(\omega_3 \pm \omega_1)].
$$
\n(20)

Their periodic dependence on ω_3 gives rise, through (19), to the periodic time dependence in (17).

These classical tilted $so(4,2)$ variables have simple geometrical meanings. Figure ¹ shows a typical orbit with the particle at P and the center of attraction at S , and the standard construction⁶ of the Kepler angle Φ ("eccentric anomaly") from the "true anomaly" Ψ . Also shown is the "mean anomaly" ω_3 , which varies linearly with the time as shown in (19) , and which changes in

FIG. 1. Typical orbit and "anomalies" for the classical problem.

value by 2π as the particle completes an orbit. It is constructed from Φ using the formula $\omega_3 = \Phi - \epsilon \sin \Phi$, where $\epsilon = (1+2HL^2/me^4)^{1/2}$ is the eccentricity of the ellipse. The ellipse in Fig. 2 has the same orientation as the orbit, but has been scaled by a factor \overline{N} ⁻¹ so that the Runge Lenz vector runs from the center to a focus S' as shown.
The construction of the time-dependent variables M^* and Γ^* is also shown in Fig. 2, where OQ and OQ' are perpendicular, and Γ_4^* , T^* are given from the figure by $\epsilon \overline{OX}, \epsilon \overline{OY}$, respectively. It follows that Γ_4^* and T^* are, apart from a factor ϵ , the Cartesian coordinates of the moving point Q , relative to the axes OX, OY through the

FIG. 2. Tilted so(4,2) variables for the classical problem in the case of a closed orbit.

center of the ellipse. From Fig. 2 we can easily see that center of the ellipse. From Fig. 2 we can easily see that each of Γ^* , M^* , T^* , and Γ_4^* is a constant multiple of $cos\omega_3$ or $sin\omega_3$, and so is periodic in time, with the same period as the particle's motion. Not shown with Fig. 2 is the (constant) angular momentum vector L, directed perpendicular to the plane of the ellipse, and the remaining so(4,2) variable, the constant

$$
\Gamma_0^* = me^2(-2mH)^{-1/2}
$$

It can be seen that these $so(4,2)$ variables are not all functionally independent: For example, the size and orientation of the orbit can be determined from L and A^* (which provide five independent constants since L A^* = 0), while the value of ω_3 , and hence the position of the particle on the orbit, can be determined by T^* (or Γ_4^*). The remaining variables Γ_0^* , Γ_4^* (or T^*), M^* , and Γ^* are then determined. In the quantum-mechanical model, the corresponding feature is the degeneracy of the representation of so(4,2) involved; in such representations not all basis operators are functionally independent. '

On the subspace corresponding to continuum states of the quantum-mechanical problem we can transform Γ_4 the quantum-mechanical problem we
into $\Gamma_4^* = K_1^{-1} \Gamma_4 K_1 = (2H)^{-1/2}$, where

$$
K_1 = \exp[iT \cdot \ln(X)] \alpha_1(X) , \qquad (21)
$$

and $X = (2H)^{-1/2} = \Gamma_4^*$, which is well defined for the unbound states. We find (in dimensionless form)

$$
\mathbf{L}^* = \mathbf{L} = \mathbf{r} \times \mathbf{p}, \quad \mathbf{M}^* = \frac{1}{2} \left[\mathbf{p} \times \mathbf{L} - \mathbf{L} \times \mathbf{p} - 2 \frac{\mathbf{r}}{r} \right] X, \quad \Gamma_4^* = X,
$$
\n
$$
\Gamma_0^* \pm T^* = \frac{1}{2} r p^2 E_{\mp} (X \mp i) + \frac{1}{2} r E_{\mp} (X \mp i)^{-1} \pm (\mathbf{r} \cdot \mathbf{p} - i) E_{\mp} ,
$$
\n
$$
\Gamma^* \pm \mathbf{A}^* = r \mathbf{p} E_{\pm} \pm [\frac{1}{2} r p^2 - (\mathbf{r} \cdot \mathbf{p} - i) \mathbf{p}] E_{\pm} (X \pm i)
$$
\n
$$
\mp \frac{1}{2} r E_{\pm} (X \pm i)^{-1} ,
$$
\n
$$
E_{\pm} = \exp\{i (\mathbf{r} \cdot \mathbf{p} - i) : \ln[X(X \pm i)^{-1}]\} \alpha_1(X)[\alpha_1(X \pm i)]^{-1}
$$

[where $\alpha_1(X)$ has to be chosen to make the tilted so(4,2) operators Hermitian, and it appears that analogously to the bound case, $\alpha_1(X)=X$] with time dependence

$$
\Gamma_0^*(t) \pm T^*(t) = [\Gamma_0^*(0) \pm T^*(0)]
$$

\n
$$
\times \exp[\mp t (X \mp \frac{1}{2}i)X^{-2}(X \mp i)^{-2}],
$$

\n
$$
\Gamma^*(t) \pm \mathbf{A}^*(t) = [\Gamma^*(0) \pm \mathbf{A}^*(0)]
$$

\n
$$
\times \exp[\pm t (X \pm \frac{1}{2}i)X^{-2}(X \pm i)^{-2}], \qquad (23)
$$

and
$$
\Gamma_4^*(-X)
$$
, **M**^{*}, and **L**^{*}(=L) are constants of the motion.

The corresponding classical variables in dimensional form are

$$
\mathbf{L}^* = \mathbf{L} = \mathbf{r} \times \mathbf{p}, \quad \Gamma_4^* = me^2 \overline{X},
$$
\n
$$
\mathbf{M}^* = [\mathbf{p} \times \mathbf{L} - me^2(\mathbf{r}/r)] \overline{X},
$$
\n
$$
\Gamma_0^* \pm T^* = \frac{1}{2} (rp^2 \overline{X} + (r/\overline{X}) \pm 2\mathbf{r} \cdot \mathbf{p}) U_1^{\mp 1},
$$
\n
$$
\Gamma^* \pm \mathbf{A}^* = [rp \pm \frac{1}{2} (rp^2 - 2(\mathbf{r} \cdot \mathbf{p}) \mathbf{p}) \overline{X} \mp \frac{1}{2} (\mathbf{r}/\overline{X})] U_1^{\pm 1},
$$
\n
$$
\overline{X} = (2mH)^{-1/2}, \quad U_1 = \exp(\mathbf{r} \cdot \mathbf{p}/me^2 \overline{X})]
$$

with time dependence

$$
\Gamma_0^*(t) \pm T^*(t) = [\Gamma_0^*(0) \pm T^*(0)] \exp(\mp t/V_1),
$$

\n
$$
\Gamma^*(t) \pm A^*(t) = [\Gamma^*(0) \pm A^*(0)] \exp(\pm t/V_1),
$$

\n
$$
V_1 = m^2 e^2 \overline{X}^3
$$

and Γ_4^* , M^* , and L are constants of the motion. The variables in (24) also have simple geometric meanings for hyperbolic and parabolic orbits.

CONCLUSION

We have shown that tilted $so(4,2)$ operators can be defined on the bound states of the Coulomb problem, with a simple time dependence which is clearly analogous to that of corresponding classical variables. These classical variables have a simple geometrical interpretation. In the quantum case, since the representation of $so(4, 2)$ on $\mathcal V$ is irreducible, all operators on $\mathcal V$ can in principle be expressed in terms of these tilted so(4,2) operators, and we can therefore claim to have effected a complete integration of Heisenberg's equations of motion for the system, at least on $\mathcal V$. The rather mysterious tilt transformation has been revealed to be, at the classical level, a transformation of the original $so(4, 2)$ variables into ones which are simple functions of action-angle variables. Corresponding results have been indicated for the unbound case.

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