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The lowest energy state for a polynomial Hamiltonian and its geometrical interpretation†

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Abstract. Consider a Hamiltonian H which is an element of the enveloping algebra of a Lie algebra \mathcal{L} . For simplicity we choose \mathcal{L} as $\mathfrak{su}(2)$ or $\mathfrak{su}(1, 1)$. We look for the coherent state $|sc\rangle$ which solves the variational equation $\delta\langle sc|H|sc\rangle = 0$. This condition in state space is transcribed into a condition in a classical phase space. Geometrical concepts are given for the state of lowest energy, and for a self-consistent linearised Hamiltonian. The interpretation yields solutions of the equation for the state of lowest energy by iteration procedures.

1. Introduction

The dequantisation of quantum mechanical problems makes it possible to study quantum dynamics in terms of classical dynamics. From the expectation values of operators with coherent states, we get classical or dequantised observables on phase spaces with generalised Poisson brackets. The Hamiltonian is an element of the enveloping algebra of a Lie algebra \mathcal{L} , and the phase spaces are hypersurfaces given by constant values of the Casimir observables, on the dual space \mathcal{L}^* to the Lie algebra.

In the present paper we derive a concept for the construction of lowest energy states and give a geometrical interpretation for all physical quantities which occur. For simplicity we choose as Lie algebra $\mathfrak{su}(2)$ or $\mathfrak{su}(1, 1)$.

Starting with a Hamiltonian H , which is at most quadratic in the basis of the Lie algebra $\mathfrak{su}(2)$ respectively an element of the enveloping algebra of $\mathfrak{su}(1, 1)$, we look for those normalised coherent states $|sc\rangle$ in an irreducible representation space of the corresponding Lie group which solve the variational equation $\delta\langle sc|H|sc\rangle = 0$. From this variational equation we derive extremal conditions which have a simple geometrical interpretation. After dequantising the Hamiltonian we construct a self-consistent linear Hamiltonian. Its geometrical interpretation is that of a plane tangent to the Hamiltonian energy surface, whereas the state $|sc\rangle$ corresponds to a particular point on this energy surface. With this interpretation we construct graphical iteration procedures and transcribe them into numerical ones. To show the geometrical content of the concept, we demonstrate the method on two instructive and solvable examples for each of the two groups.

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2. Hamiltonians based on SU(2)

In this section we construct a polynomial Hamiltonian H which is at most quadratic in the basis of the Lie algebra of SU(2) and its dequantisation.

The operators $\{J_3, J_+, J_-\}$ are the basis elements of the Lie algebra $\mathfrak{su}(2)$, which fulfil the well known commutator relations $[J_3, J_\pm] = \pm J_\pm$, $[J_+, J_-] = 2J_3$. Without loss of generality we can represent the Hamiltonian H by irreducible tensor operators J_q^k (Edmonds 1957) of maximum rank two, where k denotes the rank and q the components, $q = -k, -k + 1, \dots, +k$.

$$H = \sum_{k=0}^2 \sum_{q=-k}^{+k} a_{kq} (-1)^q J_{-q}^k. \tag{2.1}$$

From the hermiticity of the Hamiltonian we get with $(J_{-q}^k)^+ = (-1)^q J_q^k$: $\overline{a_{kq}} = (-1)^q a_{k-q}$; ‘+’ denotes the Hermitian adjoint, and ‘-’ the complex conjugate. As trial states we define the coherent states $|z\rangle$ (Perelomov 1972) of the group SU(2) (Kramer and Saraceno 1981) by

$$|z\rangle := \exp(\bar{z}J_-)|jj\rangle, \tag{2.2}$$

where $|jj\rangle$ is the highest weight state.

For an arbitrary operator A we define

$$\mathcal{A}(z', \bar{z}) := \langle z'|A|z\rangle / \langle z'|z\rangle. \tag{2.3}$$

The generalised Poisson bracket $\{.,.\}$ (Kramer and Saraceno 1981), defined by

$$\{\mathcal{F}, \mathcal{G}\} = -\frac{(1+z\bar{z})^2}{2j} \left(\frac{\partial \mathcal{F}}{\partial z} \frac{\partial \mathcal{G}}{\partial \bar{z}} - \frac{\partial \mathcal{F}}{\partial \bar{z}} \frac{\partial \mathcal{G}}{\partial z} \right) \tag{2.4}$$

for arbitrary functions $\mathcal{F}(z, \bar{z})$ and $\mathcal{G}(z, \bar{z})$, provides a Poisson realisation of the representation of the Lie algebra.

Proposition. \forall coherent states $|z\rangle$, where $J \in \mathfrak{su}(2)$ and A is an arbitrary operator

$$\{\mathcal{J}, \mathcal{A}\}(z, \bar{z}) = \langle z|[J, A]|z\rangle / \langle z|z\rangle. \tag{2.5}$$

Proof. For the proof see Kramer and Saraceno (1981).

To get numerical expressions later on, we need a suitable parametrisation of the coherent states $|z\rangle$. By the stereographic projection (Cartan 1961) of the complex plane onto the Riemann sphere one obtains

$$z = \tan \frac{1}{2}\beta \cdot \exp(-i\gamma) \quad 0 < \gamma \leq 2\pi, 0 \leq \beta \leq \pi \tag{2.6}$$

which leads to the usual spherical coordinates for $\mathcal{J}_i(\beta, \gamma) \quad i \in \{1, 2, 3\}$.

Interpretation. Consider \mathbb{R}^3 with axes labelled by $\mathcal{J}_1, \mathcal{J}_2, \mathcal{J}_3$. Then $\mathcal{J}_i(\beta, \gamma)$ is the restriction of the coordinate functions to the sphere of radius j . It is useful to consider not only this sphere, but also $\mathbb{R}^3 \sim \mathcal{L}^x \text{SU}(2)$, the dual of the Lie algebra $\mathfrak{su}(2)$. This will be fundamental for what follows. It is well known that on the dual \mathcal{L}^x of a Lie algebra there exists a degenerate Poisson bracket which yields a realisation of the Lie algebra \mathcal{L} . The Poisson bracket given above is the restriction of this degenerate bracket to a non-degenerate projection onto a sphere of radius j (Kramer and Saraceno 1981). We shall use this relation for an interpretation of the quantum dynamics in terms of

geometrical concepts of classical dynamics. From the Hamiltonian (2.1) we get with definition (2.3)

$$\mathcal{H}(z, \bar{z}) = \sum_{k=0}^2 \sum_{q=-k}^{+k} (-1)^q a_{kq} \mathcal{F}_{-q}^k(z, \bar{z}). \quad (2.7)$$

Hence, $\mathcal{H}(z, \bar{z})$ can be written as a function of \mathcal{F}_i and therefore $\mathcal{H}(\mathcal{F}) = E$ may be interpreted as the subvariety $\{\mathcal{F} = (\mathcal{F}_1, \mathcal{F}_2, \mathcal{F}_3) | \mathcal{H}(\mathcal{F}) - E = 0\}$ i.e. a two-dimensional surface in a three-dimensional space spanned by the euclidian functions \mathcal{F}_q .

Now we are able to look for those states $|sc\rangle := |z\rangle / \langle z|z\rangle^{1/2}$ which solve the variational equation $\delta\mathcal{H}(z, \bar{z}) = 0$.

Proposition.

$$\delta\mathcal{H}(z, \bar{z}) = 0 \Leftrightarrow \frac{\langle z|[J_q, H]|z\rangle}{\langle z|z\rangle} = 0 \quad \forall q \in \{3, +, -\} \quad (2.8)$$

and with proposition (2.5)

$$\{\mathcal{F}_q, \mathcal{H}\}(z, \bar{z}) = 0.$$

Proof. The variational principle $\delta\mathcal{H}(z, \bar{z}) = 0$ implies that the derivatives of \mathcal{H} with respect to z and \bar{z} vanish. Together with proposition (2.5) and the explicit form of the generalised Poisson bracket (2.4) this yields the result.

To use the equation above, we have to dequantise the Hamiltonian (2.1), which only means the transition from the Hamiltonian H to the corresponding energy surface \mathcal{H} as a function of the cartesian components of the angular momentum. For that we need the connection between \mathcal{F}_q^k (the expectation value of the irreducible tensor operators J_q^k) and the irreducible tensors $(\cdot \mathcal{F})_q^k$. Define J_q^1 with expectation value \mathcal{F}_q^1 and

$$J_q^k = [J^{k-1} J^1]_q^k, (\cdot \mathcal{F}_q^k) = [\mathcal{F}^{k-1} \mathcal{F}^1]_q^k \quad k = 1, 2, \dots$$

Theorem. For all irreducible tensor operators

$$J_r^k (k > 0): \mathcal{F}_r^k = \left(\frac{1}{2j}\right)^k (\cdot \mathcal{F})_r^k \prod_{i=0}^{k-1} (2j - 1). \quad (2.9)$$

Proof. It is clear from the transformation properties of the irreducible tensor operators J_r^k and the tensors $(\cdot \mathcal{F})_r^k$ that $(\cdot \mathcal{F})_r^k \sim \mathcal{F}_r^k$. Hence

$$\mathcal{F}_r^k = \alpha_k (\cdot \mathcal{F})_r^k \quad \forall r: -k \leq r \leq k.$$

Because of $J_k^k = N(J_+)^k$ with a normalisation constant N , we get

$$\mathcal{F}_k^k = N\mathcal{F}_+^k = \alpha_k N(\mathcal{F}_+)^k = \alpha_k (\cdot \mathcal{F})_k^k, \quad \mathcal{F}_+^k = \langle z|J_+^k|z\rangle / \langle z|z\rangle$$

$$\begin{aligned} \mathcal{F}_+^k &= \frac{1}{\langle z|z\rangle} \frac{\partial^k}{\partial z^k} \langle z|z^k\rangle |_{z=z} \\ &= \bar{z}^k (1 + z\bar{z})^k \prod_{l=0}^{k-1} (2j - 1) \\ &= (\cdot \mathcal{F}_+^k) \left(\frac{1}{2j}\right)^k \prod_{l=0}^{k-1} (2j - 1). \end{aligned}$$

Now we are able to write \mathcal{H} explicitly as a function of \mathcal{F}_i and define for convenience

$$\mathcal{H}(\mathcal{F}_1, \mathcal{F}_2, \mathcal{F}_3) =: \sum_{i=1}^3 b_i \mathcal{F}_i + \sum_{i \leq j=1}^3 c_{ij} \mathcal{F}_i \mathcal{F}_j, \tag{2.10}$$

but notice that the coefficients c_{ij} depend on j .

Interpretation. Consider \mathcal{H} as a classical Hamiltonian defined on \mathbb{R}^3 , even if the coefficients depend on j . It determines energy surfaces in \mathbb{R}^3 such that $\mathcal{H}(z, \bar{z})$ yields the values of \mathcal{H} when restricted to the sphere. Then proposition (2.8) requires that the energy and angular momentum surfaces have the same tangential plane at the intersection point.

3. Self-consistency and its geometrical interpretation

To give a geometrical picture for the extremal conditions above, we define a self-consistent linear Hamiltonian H_{sc} by

$$\langle sc | H_{sc} | sc \rangle = \langle sc | H | sc \rangle \tag{3.1}$$

and

$$\langle sc | [J_q, H_{sc}] | sc \rangle = \langle sc | [J_q, H] | sc \rangle \quad \forall q \in \{1, 2, 3\}, \tag{3.2}$$

and this is a nonlinear equation like the Hartree–Fock equations (Matsen 1978).

Because H_{sc} is a linear operator in the Lie algebra

$$\mathcal{H}_{sc}^{(z)}(z, \bar{z}) := \langle z | H_{sc} | z \rangle / \langle z | z \rangle \tag{3.3}$$

is a linear function in \mathcal{F}_i and therefore determines a plane in a space spanned by the cartesian components \mathcal{F}_i of the angular momentum. The equations corresponding to the quantum mechanical conditions (3.1), (3.2) are

$$\mathcal{H}_{sc}^{(z)}(z, \bar{z}) = \mathcal{H}(z, \bar{z}) \tag{3.4}$$

and

$$\{\mathcal{F}_q, \mathcal{H}\}(z, \bar{z}) = \{\mathcal{F}_q, \mathcal{H}_{sc}^{(z)}\}(z, \bar{z}), \tag{3.5}$$

where we have made use of proposition (2.5). These two equations have only a local validity. For convenience we define

$$\mathcal{H}_{sc}^{(z)} := \sum_{i=1}^3 \beta_i^{(z)} \mathcal{F}_i \tag{3.6}$$

and use (2.10), hence

$$\begin{aligned} 0 &= \left\{ \mathcal{F}_q, \sum_i (b_i \mathcal{F}_i - \beta_i^{(2)} \mathcal{F}_i) + \sum_{i,j} c_{ij} \mathcal{F}_i \mathcal{F}_j \right\} \\ &= i \cdot \sum_k \sum_j \left(b_j + 2 \sum_i c_{ij} \mathcal{F}_i - \beta_j^{(2)} \right) \epsilon_{qjk} \mathcal{F}_k \end{aligned}$$

and consequently

$$\beta_j^{(z)} = \sum_i \left(b_j + 2 \sum_i c_{ij} \mathcal{F}_i \right) = \frac{\partial \mathcal{H}}{\partial \mathcal{F}_i}(z, \bar{z}).$$

We obtain the geometrical interpretation summarised below.

(1) (3.4) requires a common point of the plane $\mathcal{H}_{sc}^{(z)} = E$ with the energy surface $\mathcal{H} = E$.

(2) (3.5) requires that $\mathcal{H}_{sc}^{(z)} = E$ determines a plane tangent to the energy surface at (z, \bar{z}) ,

i.e. $\{\mathcal{H}_{sc}^{(z)} | z \in \mathbb{C}\}$ contains all possible tangent planes and $\mathcal{H}_{sc}^{(z)}(z, \bar{z})$ determines a vector from the origin to the energy surface \mathcal{H} at (z, \bar{z}) . The self-consistent Hamiltonian \mathcal{H}_{sc} has to fulfil in addition the extremal conditions, hence it is a special element from the set above. After this interpretation we shall omit the index $^{(z)}$ in the following.

From the extremal condition we get

$$\{\mathcal{F}_q, \mathcal{H}_{sc}\} = 0 \tag{3.7}$$

and, hence, $\mathcal{H}_{sc} = E$ determines a plane tangent to the sphere too. Thus, \mathcal{H}_{sc} determines the tangential plane at the point of contact of the energy surface with the angular momentum sphere. The self-consistent state $|sc\rangle$ is then that state which corresponds to this point of contact.

$$\mathcal{H}_{sc}(\mathcal{F}) = \mathcal{H}(\mathcal{F}^s) - \sum_{j=1}^3 (\mathcal{F}_j^s - \mathcal{F}_j) \frac{\partial \mathcal{H}}{\partial \mathcal{F}}(\mathcal{F}^s), \tag{3.8}$$

where 's' denotes the point of contact.

By a finite SU(2)-transformation one gets a standard form of \mathcal{H} , which characterises the energy surface. The invariants for this characterisation are labelled in Bronstein and Semendjajew (1973).

4. The iteration procedure

Before constructing a graphical iteration procedure, we discuss how the energy surfaces vary, if the energy changes. All non-parabolic surfaces are described in the form

$$\sum_i \frac{\alpha_i}{E} (\mathcal{F}_i - \mathcal{F}_{i,0})^2 = 1.$$

Therefore, a change of the energy means a change of the principal axes of the energy surface while keeping its centre, and this, essentially, corresponds to a swell or a shrink of the surface.

All parabolic surfaces are represented in the form

$$\sum_{i \neq j} \alpha_i (\mathcal{F}_i - \mathcal{F}_{i,0})^2 \pm (\mathcal{F}_j - \mathcal{F}_{j,0} - E) = 0,$$

which means only a translation along the axis \mathcal{F}_j without change of shape, if the energy varies. From (3.4, 5 and 7) and their interpretation we get two possible iteration procedures; in what follows labelled by A and B.

(A) The energy-surface and the angular momentum sphere are drawn cutting each other. The tangential plane to the energy surface at an arbitrary point of intersection is then constructed. Now, by parallel shifting of this plane, a tangential plane to the sphere is constructed. In the sense given above, the energy surface is altered, until it cuts the sphere at the tangential point and the tangent plane to the energy surface is again constructed at this point. The whole procedure is repeated until the point of contact sphere–energy surface is constructed.

(B) As in (A), the energy surface and the angular momentum sphere are drawn cutting each other. But now we start with a tangent plane to the sphere at an arbitrary point of the intersection and construct a parallel tangential plane at the energy surface. The tangential point along the radius vector is projected onto the sphere and the energy surface altered so that it cuts the sphere at this projected point. Now the whole procedure is repeated until the point of contact is constructed. To obtain numerical expressions for the iteration, we use the parametrisation of § 2 for the coherent states $|z\rangle$.

For convenience we define

$$\frac{1}{j} \cdot b_i =: c_i \quad i \in \{1, 2, 3\} \tag{4.1}$$

and obtain from equation (3.7) and (3.8), for the first iteration process (A)

$$\tan \gamma_{i+1} = -\frac{c_2 + c_{12} \sin \beta_i \cos \gamma_i - 2c_{22} \sin \beta_i \sin \gamma_i - c_{23} \cos \beta_i}{c_1 + 2c_{11} \sin \beta_i \cos \gamma_i - c_{12} \sin \beta_i \sin \gamma_i - c_{13} \cos \beta_i} \tag{4.2}$$

$$\tan \beta_{i+1} = -\left(\frac{c_1 + 2c_{11} \sin \beta_i \cos \gamma_i - c_{12} \sin \beta_i \sin \gamma_i - c_{13} \cos \beta_i}{c_3 + c_{13} \sin \beta_i \cos \gamma_i - c_{23} \sin \beta_i \sin \gamma_i - 2c_{33} \cos \beta_i}\right) \left(\frac{1}{\cos \gamma_{i+1}}\right) \tag{4.3}$$

$$\tan \beta_{i+1} = +\left(\frac{c_2 + c_{12} \sin \beta_i \cos \gamma_i - 2c_{22} \sin \beta_i \sin \gamma_i - c_{23} \cos \beta_i}{c_3 + c_{13} \sin \beta_i \cos \gamma_i - c_{23} \sin \beta_i \sin \gamma_i - 2c_{33} \cos \beta_i}\right) \left(\frac{1}{\sin \gamma_{i+1}}\right) \tag{4.4}$$

where the indices $i, i+1$ label the iteration. In a similar way one derives equations for iteration process (B).

5. Examples

We will demonstrate the method by two solvable examples. For the first one we choose the ellipsoid as a non-parabolic energy surface. The physical background is for example the force-free rigid body. As an example for a parabolic energy surface we choose the Lipkin model (Glick *et al* 1961, Lipkin *et al* 1965, Agassi *et al* 1966). The Lipkin model is an N -fermion system distributed into two entirely degenerate energy levels. The Hamiltonian for the ellipsoid is

$$\begin{aligned} \mathcal{H} &= c_{11}\mathcal{I}_1^2 + c_{22}\mathcal{I}_2^2 + c_{33}\mathcal{I}_3^2 \\ &= j^2(c_{11} \sin^2 \beta \cos^2 \gamma + c_{22} \sin^2 \beta \sin^2 \gamma + c_{33} \cos^2 \beta) \end{aligned} \tag{5.1}$$

with $c_{ii} > 0$ for the real and $c_{ii} < 0$ for the imaginary ellipsoid (negative energy).

For the iteration procedure (A) we get from (4.2) and (4.3)

$$\tan \gamma_{i+1} = \frac{c_{22}}{c_{11}} \tan \gamma_i \tag{5.2}$$

$$\tan \beta_{i+1} = \frac{c_{22} \sin \gamma_i}{c_{33} \sin \gamma_{i+1}} \cdot \tan \beta_i \tag{5.3}$$

or

$$\tan \gamma_\infty = \lim_{n \rightarrow \infty} \left(\frac{c_{22}}{c_{11}}\right)^n \cdot \tan \gamma_0$$

and

$$\tan \beta_{i+1} = \tan \beta_i \cdot \left(\frac{(c_{11}/c_{33})^2 + (c_{22}/c_{33})^2 \tan^2 \gamma_i}{1 + \tan^2 \gamma_i} \right)^{1/2}.$$

Explicit discussion of these equations shows the iteration (A) going always to the energy maximum (minimum) for the real (imaginary) ellipsoid. For the iteration procedure (B) it follows that

$$\tan \gamma_{i+1} = \frac{c_{11}}{c_{22}} \tan \gamma_i \tag{5.4}$$

$$\tan \beta_{i+1} = \frac{c_{33}}{c_{22}} \frac{\sin \gamma_i}{\sin \gamma_{i+1}} \tan \beta_i. \tag{5.5}$$

The comparison with the previous equations shows the opposite behaviour; this iteration goes always to the energy minimum (maximum) for the real (imaginary) ellipsoid. The graphical iteration procedure is drawn in figure 1.

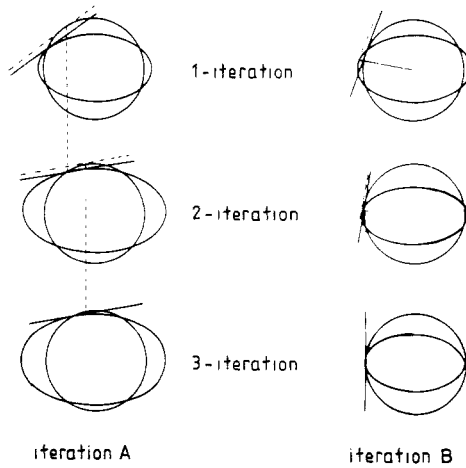


Figure 1. Iteration example for an elliptic energy surface.

The Hamiltonian for the Lipkin model is

$$H = \epsilon J_3 - \frac{1}{2} \mathcal{V} (J_+^2 + J_-^2) \tag{5.6}$$

where \mathcal{V} is a parameter for the strength of the interaction, and J_i are the quasi-spin operators. Hence the equation for the energy surface is

$$\mathcal{H} = \mathcal{J}_3 - \frac{2j-1}{2j} \mathcal{V} (\mathcal{J}_1^2 - \mathcal{J}_2^2) \tag{5.7}$$

and this is a hyperbolic paraboloid. With

$$\chi := (\mathcal{V}/\epsilon)(2j-1) \tag{5.8}$$

we get

$$(1/\epsilon j) \mathcal{H}(\beta, \gamma) = \cos \beta - \frac{1}{2} \chi \sin^2 \beta \cdot \cos 2\gamma. \tag{5.9}$$

If we measure the energy in $E/\epsilon j$ the only remaining parameter is χ , which completely

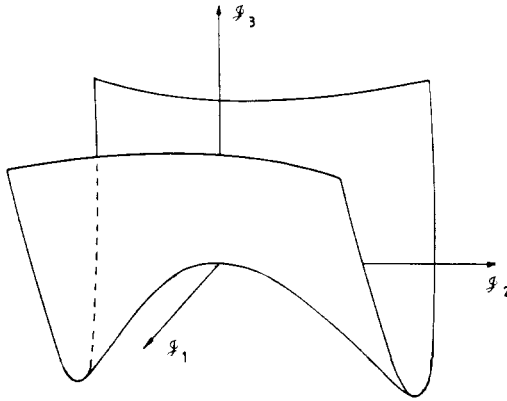


Figure 2. Energy surface of the Lipkin model (5.7).

determines the energy surface. For the iteration (A) we get

$$\tan \gamma_{i+1} = -\tan \gamma_i \tag{5.10}$$

$$\tan \beta_{i+1} = -\chi \cdot \sin \beta_i \tag{5.11}$$

and for (B)

$$\tan \gamma_{i+1} = -\tan \gamma_i \tag{5.12}$$

$$\sin \beta_{i+1} = \frac{1}{\chi} \tan \beta_i \frac{\sin \gamma_i}{\sin \gamma_{i+1}} = -\frac{1}{\chi} \tan \beta_i. \tag{5.13}$$

Equations (5.10) and (5.12) make sense only if $\gamma_i = \gamma_0 = 0$ or $\frac{1}{2}\pi \text{ mod } \pi$. Because $\mathcal{H}(\beta, \gamma) = \mathcal{H}(\beta, \gamma + \pi)$ it is sufficient to examine only the case $\gamma_i = 0, \frac{1}{2}\pi$. The only interesting iteration procedure is (A), because for the iteration (B) equation (5.13) enforces $\lim_{i \rightarrow \infty} \beta_i = 0$, which is never an energy minimum.

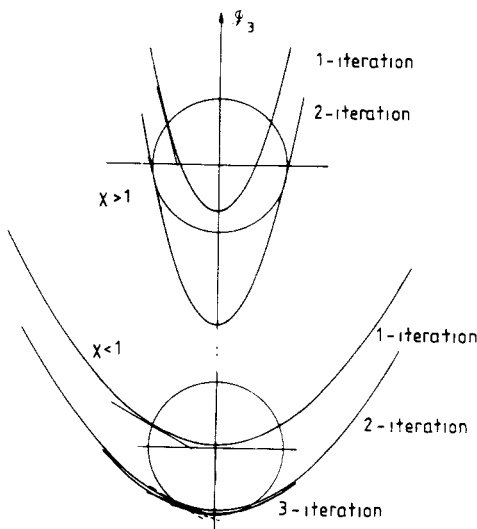


Figure 3. Iteration example for the Lipkin model.

The iteration equations (5.10) and (5.11) show a phase transition at $\chi = 1$. For $\chi \leq 1$ the energy minimum lies always at $\beta = \pi$ and for $\chi > 1$ at $\beta \neq \pi$. The geometrical viewpoint, we prefer in this paper, yields these facts in a simple way.

Finally we show the graphical iteration procedure in figure 3.

6. Hamiltonians based on SU(1, 1)

The case where the Hamiltonian is quadratic in the generators of the group SU(1, 1) is very similar to the one discussed before. One would get directly most of the following formulae, by trimming with the factor $(-i)$. Nevertheless, there are important differences, for example, the metric. If we bear these facts in mind, it is safe to assume analogous geometrical interpretations. The physical reason for our interest is the possibility of studying Hamiltonians with central potentials (Kramer 1981), but also for example the Foldy model for a superfluid Bose system, like ^4He (Solomon 1971), well known in solid state physics.

We choose as a basis for the Lie algebra

$$[A_3, A_{\pm}] = \pm A_{\pm} \quad [A_+, A_-] = -2A_3. \tag{6.1}$$

By using

$$\begin{aligned} A_0^0 &= A_3^2 - A_1^2 - A_2^2 \\ A_{\pm 1}^1 &= \pm \sqrt{1/2} i A_{\pm}, \quad A_0^1 = A_3 \\ A_{\pm 2}^2 &= -\frac{1}{2} \sqrt{3/2} A_{\pm}^2, \dots \end{aligned} \tag{6.2}$$

we get the general quadratic Hamiltonian H

$$H = \sum_{k=0}^2 \sum_{q=-2}^{+2} a_{kq} (-1)^q A_{-q}^k. \tag{6.3}$$

As $(A_{-q}^k)^+ = A_q^k$, the hermiticity of the Hamiltonian requires

$$\overline{a_{kq}} = a_{k-q}. \tag{6.4}$$

To consider the dequantised Hamiltonian we define the coherent states by (Kramer and Saraceno 1981)

$$|z\rangle := \exp(\bar{z}A_+) |qq\rangle, \tag{6.5}$$

where $|qq\rangle$ is the lowest weight state. For the numerical calculations later on we need a suitable parametrisation for the coherent states $|z\rangle$, which we choose to be

$$z = i \cdot \tanh \frac{1}{2} \beta \cdot \exp(-i\alpha). \tag{6.6}$$

In order to get the corresponding energy surface \mathcal{H} , we need again the connection between the expectation value of the irreducible tensor operators and the irreducible tensors $(\cdot \mathcal{A})_q^k$, defined in the same way as in § 2. In analogy to theorem (2.9) we get

$$\mathcal{A}_r^k = \frac{1}{(2q)^k} (\cdot \mathcal{A})_r^k \cdot \prod_{l=0}^{k-1} (2q+l). \tag{6.7}$$

Hence from (6.3) $\mathcal{H}(\mathcal{A}_1, \mathcal{A}_2, \mathcal{A}_3)$, which we define for convenience as

$$\mathcal{H}(\mathcal{A}_1, \mathcal{A}_2, \mathcal{A}_3) =: \sum_{i=1}^3 b_i \mathcal{A}_i + \sum_{i \leq j=1}^3 c_{ij} \mathcal{A}_i \mathcal{A}_j. \tag{6.8}$$

From (6.6) and (2.3) follows

$$\mathcal{A}_0^0 = \mathcal{A}_3^2 - \mathcal{A}_1^2 - \mathcal{A}_2^2 = q^2. \tag{6.9}$$

7. The iteration

The graphical iteration can be derived from (6.8) and (6.9). Energy conservation requires the components \mathcal{A}_i to run only on the energy surface $\mathcal{H}(\mathcal{A}_1, \mathcal{A}_2, \mathcal{A}_3) = E = \text{constant}$. Equation (6.9) defines a two-sheeted hyperboloid and, therefore, the only possible solutions are the cutting lines of these two hyperplanes. The general quantum mechanical conditions for the self-consistent state derived in § 4 are independent of the chosen group. With the preliminary remarks of § 6 we get the following picture.

$\mathcal{H}(\mathcal{A}) = E$ can be interpreted as an energy surface in the Minkowski space spanned by the three pseudo-euclidian components \mathcal{A}_i . The self-consistent state corresponds to the point of contact of this energy surface with the hyperboloid $\mathcal{A}_3^2 - \mathcal{A}_1^2 - \mathcal{A}_2^2 = \text{constant}$. If the hyperboloid \mathcal{A}_0^0 take the place of the sphere $\mathcal{F}_0^0 = \mathcal{F}^2$ the two graphical iteration procedures are the same as in § 5, and therefore labelled with (A) and (B) too.

To derive the iteration equations, we define the linearised Hamiltonian

$$\mathcal{H}_{sc} := \mathcal{H}(\mathcal{A}^s) - \sum_{i=1}^3 \frac{\partial \mathcal{H}(\mathcal{A}^s)}{\partial \mathcal{A}_i} (\mathcal{A}_i^s - \mathcal{A}_i). \tag{7.1}$$

For convenience we define

$$(1/q)b_i =: c_i \quad i \in \{1, 2, 3\} \tag{7.2}$$

and get with the extremal condition $\{\mathcal{A}_i, \mathcal{H}_{sc}\} = 0$ for iteration (A)

$$\begin{aligned} & \tanh \beta_{i+1} \cdot \cos \alpha_{i+1} \\ &= \frac{c_2 + c_{12} \sinh \beta_i \cdot \sin \alpha_i - 2c_{22} \sinh \beta_i \cdot \cos \alpha_i + c_{23} \cosh \beta_i}{c_3 + c_{13} \sinh \beta_i \cdot \sin \alpha_i - c_{23} \sinh \beta_i \cdot \cos \alpha_i + 2c_{33} \cosh \beta_i} \end{aligned} \tag{7.3}$$

$$\begin{aligned} & - \tanh \beta_{i+1} \cdot \sin \alpha_{i+1} \\ &= \left(\frac{c_1 + 2c_{11} \sinh \beta_i \cdot \sin \alpha_i - c_{12} \sinh \beta_i \cdot \cos \alpha_i + c_{13} \cosh \beta_i}{c_3 + c_{13} \sinh \beta_i \cdot \sin \alpha_i - c_{23} \sinh \beta_i \cdot \cos \alpha_i + 2c_{33} \cosh \beta_i} \right) \end{aligned} \tag{7.4}$$

$$\tan \alpha_{i+1} = - \frac{c_1 + 2c_{11} \sinh \beta_i \cdot \sin \alpha_i - c_{12} \sinh \beta_i \cdot \cos \alpha_i + c_{13} \cosh \beta_i}{c_2 + c_{12} \sinh \beta_i \cdot \sin \alpha_i - 2c_{22} \sinh \beta_i \cdot \cos \alpha_i + c_{23} \cosh \beta_i} \tag{7.5}$$

where the indices $i, i + 1$ label the iteration. In a similar way one can derive equations for iteration process (B).

8. Examples

To get a physical interpretation not only for the hyperboloid \mathcal{A}_0^0 but also for the following two examples, we introduce the boson creation and annihilation operators

a_j^+ and a_j of a system of two particles with relative coordinates x and momenta p

$$\begin{aligned} a_j^+ &:= \sqrt{1/2}(x_j - ip_j) \\ a_j &:= \sqrt{1/2}(x_j + ip_j) \quad \hbar = 1; \end{aligned}$$

then the generators A_i become

$$\begin{aligned} A_3 &= \frac{1}{4} \sum_{j=1}^3 (p_j p_j + x_j x_j), & A_1 &= \frac{1}{4} \sum_{j=1}^3 (x_j x_j - p_j p_j), \\ A_2 &= \frac{1}{4} \sum_{j=1}^3 (x_j p_j + p_j x_j). \end{aligned} \tag{8.1}$$

The angular momentum operator is

$$L_k = \sum_{j,l} \varepsilon_{kjl} \cdot x_j p_l$$

where ε_{kjl} is the Levi-Civita symbol, antisymmetric in all pairs of indices kj and jl and normalised so that $\varepsilon_{123} = 1$.

Hence, the dequantised squared angular momentum is

$$\mathcal{L}^2 = 4(\mathcal{A}_3^2 - \mathcal{A}_1^2 - \mathcal{A}_2^2) \tag{8.2}$$

and therefore, the hyperboloid \mathcal{A}_0^0 does not correspond to the quantum mechanical eigenvalue $l(l+1)$ but to the classical value l^2 .

For a local central potential, the Hamiltonian is

$$\begin{aligned} \mathcal{H} &= (1/2m) p \cdot p + V(x \cdot x) \\ &= (1/2m) \cdot 2(\mathcal{A}_3 + \mathcal{A}_1) + V(2(\mathcal{A}_3 - \mathcal{A}_1)). \end{aligned} \tag{8.3}$$

Because \mathcal{H} is independent of \mathcal{A}_2 , the corresponding energy surfaces are cylinders or planes. The harmonic oscillator is

$$\mathcal{H} = (1/m)(\mathcal{A}_3 + \mathcal{A}_1) + \alpha(\mathcal{A}_3 - \mathcal{A}_1),$$

hence a plane and for our purpose not very interesting. As a first example we regard the anharmonic quadric oscillator

$$\mathcal{H} = \frac{1}{m}(\mathcal{A}_3 + \mathcal{A}_1) + \beta(\mathcal{A}_3 - \mathcal{A}_1)^2. \tag{8.4}$$

With

$$x = \sqrt{1/2}(\mathcal{A}_3 + \mathcal{A}_1) \quad y = \sqrt{1/2}(\mathcal{A}_3 - \mathcal{A}_1) \tag{8.5}$$

(8.4) becomes

$$\mathcal{H} = \sqrt{1/2} qcx + b \cdot y^2 \quad c > 0, \tag{8.6}$$

a parabolic cylinder.

From (7.3)–(7.5) we get for the iteration procedure A

$$\tanh \beta_{i+1} \cos \alpha_{i+1} = 0 \tag{8.7}$$

and

$$-\tanh \beta_{i+1} \sin \alpha_{i+1} = \frac{c + b \sinh \beta_i \sin \alpha_i - b \cosh \beta_i}{c - b \sinh \beta_i \sin \alpha_i + b \cosh \beta_i}. \tag{8.8}$$

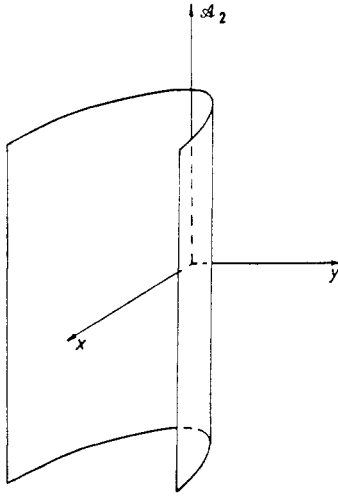


Figure 4. Energy surface of the anharmonic oscillator (8.6).

Hence $\alpha_{i+1} = \frac{1}{2}\pi \text{ mod } \pi$ and (8.8) becomes

$$\tanh \beta_{i+1} = -\frac{1 - \chi \exp(-\beta_i)}{1 + \exp(-\beta_i)} \quad \chi = \frac{b}{c} \tag{8.9}$$

for $\alpha_{i+1} = \frac{1}{2}\pi$, which is sufficient because $E(\frac{1}{2}\pi, \beta_i) = E(\frac{3}{2}\pi, -\beta_i)$. (8.7) converges only if $\chi > 0$ and this is physically and geometrically easy to understand. $\chi > 0$ means that the leg of the potential $V = b \cdot y^2$ is opened upwards, therefore, a test particle is locked in and can only oscillate about its position of equilibrium. In the opposite case $\chi < 0$, the test particle escapes to infinity. The exact solution is $\beta_\infty = \frac{1}{3} \ln \chi$, which is always a minimum. It follows graphically (see figure 6) and numerically, that the second iteration procedure (B) has no solution. The last example is not quadratic in the Lie algebra of $SU(1, 1)$ but a central force problem too—the Coulomb interaction $V(x) \sim 1/|x|$. Therefore, we cannot use the iteration equations above, we have to derive new ones.

With the Hamiltonian

$$\begin{aligned} \mathcal{H} &= a(\mathcal{A}_3 + \mathcal{A}_1) + b(\mathcal{A}_3 - \mathcal{A}_1)^{-1/2} \quad a > 0 \\ &= 2ax + 2^{-1/4} \cdot b\sqrt{1/y} \end{aligned} \tag{8.10}$$

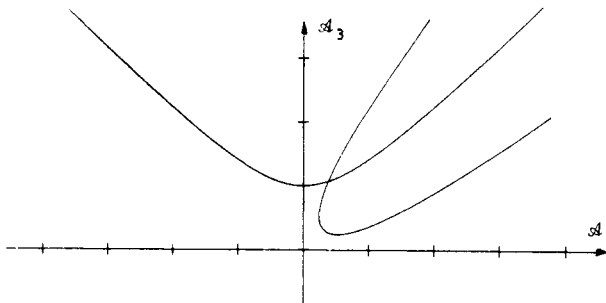


Figure 5. Cut in the \mathcal{A}_3 - \mathcal{A}_1 plane for the quadratic oscillator $\chi < 0$.

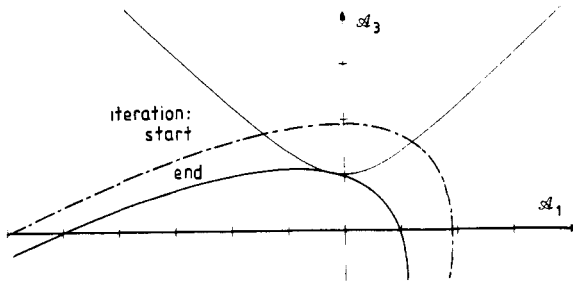


Figure 6. Cut in the $\mathcal{A}_3 - \mathcal{A}_1$ plane for the quadratic oscillator $\chi = 0$. If one constructs a tangent to the hyperboloid at the point of intersection, it can be seen that iteration procedure (B) has no solution because there exists no tangent to the energy surface which is parallel to the one above, whereas the iteration procedure (A) runs very well.

and (7.1) and the extremal condition $\{\mathcal{A}_i, \mathcal{H}_{sc}\} = 0$, the iteration equations are

$$0 = \mathcal{A}_2^{(j)}(a + \frac{1}{2}b(\mathcal{A}_3^{(i)} - \mathcal{A}_1^{(i)})^{-3/2}) \tag{8.11}$$

$$0 = \mathcal{A}_3^{(j)}(a + \frac{1}{2}b(\mathcal{A}_3^{(i)} - \mathcal{A}_1^{(i)})^{-3/2}) + \mathcal{A}_1^{(j)}(a - \frac{1}{2}b(\mathcal{A}_3^{(i)} - \mathcal{A}_1^{(i)})^{-3/2}) \tag{8.12}$$

$$0 = \mathcal{A}_2^{(j)}(a - \frac{1}{2}b(\mathcal{A}_3^{(i)} - \mathcal{A}_1^{(i)})^{-3/2}). \tag{8.13}$$

For convenience we define

$$\chi := \frac{1}{2}q^{-3/2}b/a \tag{8.14}$$

and get $\alpha = \frac{1}{2}\pi \text{ mod } \pi$ for both iteration procedures. With the same argument as in the first example we restrict the discussion to $\alpha = \frac{1}{2}\pi$. Hence for the iteration procedure (A)

$$\tanh \beta_{i+1} = -\frac{1 + \chi(\cosh \beta_i + \sinh \beta_i)^{3/2}}{1 - \chi(\cosh \beta_i + \sinh \beta_i)^{3/2}} \tag{8.15}$$

and for (B)

$$\exp(\frac{3}{2}\beta_{i+1}) = -\frac{1}{\chi} \cdot \exp(2\beta). \tag{8.16}$$

Both iteration procedures lead to the exact value $\beta_\infty = 2 \cdot \ln(-\chi)$, which is always a minimum, and converges only for $\chi < 0$ (see figure 8). This behaviour is easy to understand if we contemplate the potential $V(|x|) = b \cdot 2^{-1/4} \cdot y^{-1/2}$. For $\chi < 0$ we

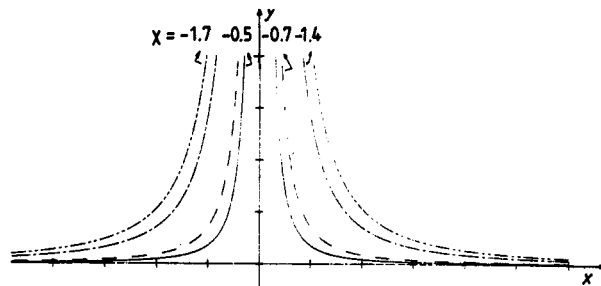


Figure 7. Cut through the energy surface of the Coulomb model (8.10).

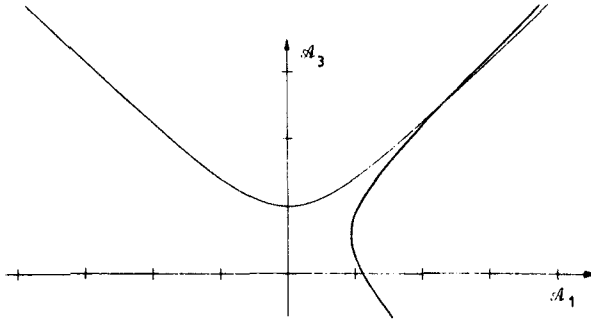


Figure 8. The figure shows that for the Coulomb model with $\chi < 0$ the energy surface has no point of contact with the hyperboloid

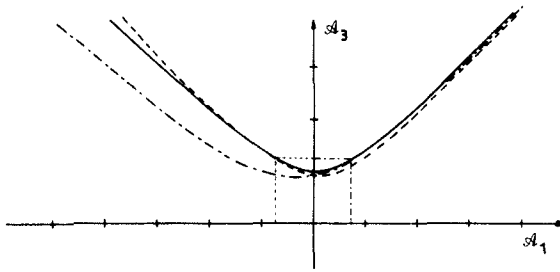


Figure 9. Iteration (A) example for the Coulomb model; hyperboloid \mathcal{A}_0^0 ; — energy surface; --- $\chi = -0.7$, - · - · - $\chi = -1.4$. The point of contact for $\chi = -a \in \mathbb{R}^+$ can be constructed from that for $\chi = -1/a$ by reflection in the mirror plane $\mathcal{A}_1 = 0$.

always have $b < 0$ and *vice versa*. If we interpret V as a Coulomb potential, $b < 0$ means e.g. the motion of an electron in the field of a nucleus. In this case bound states are possible, whereas $b > 0$ describes the motion of a charged particle in the field of a particle with the same charge, hence an unstable system. Finally we show a cut through the normalised cylindrical energy surface \mathcal{H}/aq for different χ -values and some iteration examples.

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