The Pauli Principle for Two Particles in a Dequantization Scheme Based on Coherent States

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The expectation values of operators in state space between symmetrized or antisymmetrized coherent states associated with the Weyl group are introduced as classical functions. The dequantization scheme provided by these functions yields an interpretation of permutational symmetry for classical trajectories. The two-nucleon system is treated as an example.

Introduction

The dequantization scheme developed in [1] is modified in the present paper to incorporate the orbital symmetry for a system of two particles. Classical functions on phase space are introduced as expectation values of operators between symmetrized coherent states of the Weyl group. The equations of motion are derived from the time-dependent variational principle. An analysis of the classical trajectories in phase space shows that the symmetrized or antisymmetrized states correspond to pairs of trajectories whose points are connected by the classical permutation operation. Specific examples are given for a system of two nucleons with an effective interaction.

1. Dequantization with the TDVP

We maintain the Pauli principle in the dequantization procedure by using symmetrized or antisymmetrized states respectively to compute the classical functions. The method is justified by the time-dependent variational principle (TDVP) as analyzed by Kramer and Saraceno [2]. The main features we will report here briefly. The fundamental assumption is in our case that the time-dependence of the states can be described by a complex parameter $z(t) \in \mathbb{C}^n$, and by a parametrized state $|\psi(t)\rangle = |\psi(z(t))\rangle$.

1.1 Definition

1. $\mathfrak{N}(z', \bar{z}) = \langle\psi(z')|\psi(z)\rangle$ is the normalization kernel.
2. $\mathfrak{H}(z, \bar{z}) = \langle\psi(z)|H|\psi(z)\rangle / \mathfrak{N}(z, \bar{z})$ is the classical function for the Hamiltonian operator H.
3. For every linear operator O we define the classical function by $\mathfrak{O}(z, \bar{z}) = \langle\psi(z)|O|\psi(z)\rangle / \mathfrak{N}(z, \bar{z})$.

The function $\mathfrak{H}(z, \bar{z})$ plays the role of the classical Hamiltonian. Definition 1.1 is a generalization of definition 1.10 in [1].

For the sake of simplicity we denote the scalar product by zz, $z\bar{z}$ and $\bar{z}\bar{z}$ respectively. With Z we mean the vector operator and with $\mathfrak{Z}$ the corresponding vector function.

1.2 Proposition

1. For the complex parameters the TDVP yields the equations of motion

$$\dot{z} = i\{\mathfrak{H}, z\} \quad \text{and} \quad \dot{\bar{z}} = i\{\mathfrak{H}, \bar{z}\},$$

where the generalized Poisson bracket for two functions f, g is

$$\{f, g\} = \sum_{k,l} (\partial f/\partial \bar{z}_k)(C^{-1})_{kl}(\partial g/\partial z_l) - (\partial f/\partial z_k)({}^tC^{-1})_{kl}(\partial g/\partial \bar{z}_l)$$

and the matrix C is

$$C_{kl}(z, \bar{z}) = (\partial^2/\partial z_k \, \partial \bar{z}_l) \ln \mathfrak{N}(z, \bar{z}).$$

2. On the trajectories $z(t)$, the energy $\mathfrak{H}(z, \bar{z})$ is constant, which implies that they must coincide with lines of fixed energy.

As we will work in Bargmann space $\mathfrak{B}$ we use the same decomposition of the complex variable z as in [1] and

$$z = (1/2)^{1/2}(x/b - i\,p\,b/\hbar),$$

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where $b = (\hbar/m\omega)^{1/2}$ is the oscillator constant. This leads us to functions on phase space: $\mathfrak{O}(z, \bar{z}) \to \mathfrak{o}(x, p, \hbar)$. Our main interest will be the energy-hypersurfaces on phase space, which will contain the possible trajectories.

1.3 Example:

We consider the coherent states in $\mathfrak{B}$ as parameter states. $|\psi(z)\rangle = |e_z\rangle$. The normalization kernel is $\mathfrak{N}(z', \bar{z}) = \exp(z' \; \bar{z})$. Therefore $C_{kl}(z, \bar{z}) = \delta_{kl}$, i.e. $C = 1$. The generalized Poisson bracket becomes

$$\{f, g\} = \sum_{k=1}^{n} (\partial f/\partial \bar{z}_k)(\partial g/\partial z_k) - (\partial f/\partial z_k)(\partial g/\partial \bar{z}_k).$$

This is just the first term of the generalized Moyal bracket of definition 1.17 in [1], which shows that the TDVP is the Poisson approximation for this case.

The equations of motion are finally

$$\dot{z}_l = i\{\mathfrak{H}, z_l\} = i(\partial \mathfrak{H}/\partial z_l).$$

From now on we study the relative motion of two particles. The relative vector z contains the relative distance x and the relative momentum p. This enables us to introduce three types of classical functions.

1.4 Definition:

1. $\mathfrak{O}^c(z, \bar{z}) = \langle e_z | O | e_z\rangle / \langle e_z | e_z\rangle$.
2. $\mathfrak{O}^s(z, \bar{z}) = \langle e_z^s | O | e_z^s\rangle / \langle e_z^s | e_z^s\rangle$, where $|e_z^s\rangle = (|e_z\rangle + |e_{-z}\rangle)/2$ are the symmetrized coherent states.
3. $\mathfrak{O}^a(z, \bar{z}) = \langle e_z^a | O | e_z^a\rangle / \langle e_z^a | e_z^a\rangle$, where $|e_z^a\rangle = (|e_z\rangle - |e_{-z}\rangle)/2$ are the antisymmetrized coherent states.

1.5 Proposition:

For dequantization with coherent states the trajectories $z(t)$ are the classical functions of the oscillator creation operator Z in $\mathfrak{B}$.

Proof:

$$\langle e_z | Z | e_z\rangle = z\langle e_z | e_z\rangle \quad \text{and} \quad \mathfrak{Z}^c(z, \bar{z}) = z.$$

In the following we study the other two cases in more detail.

1.6 Proposition:

For $n = 3$ the equations of motion are

1. $$\dot{z}_l = i \coth(z\bar{z}) \sum_{k=1}^{3} (\delta_{kl} - \bar{z}_k z_l / (z\bar{z} + \cosh(z\bar{z}) \sinh(z\bar{z})))(\partial \mathfrak{H}^s/\partial \bar{z}_k)$$

for symmetric dequantization and

2. $$\dot{z}_l = i \tanh(z\bar{z}) \sum_{k=1}^{3} (\delta_{kl} - \bar{z}_k z_l / (z\bar{z} - \cosh(z\bar{z}) \sinh(z\bar{z})))(\partial \mathfrak{H}^a/\partial \bar{z}_k)$$

for antisymmetric dequantization.

Proof:

According to proposition 1.2 the equations of motion are

$$\dot{z}_l = i\{\mathfrak{H}, z_l\} = i \sum_{k=1}^{3} (C^{-1}(z, \bar{z}))_{kl}(\partial \mathfrak{H}/\partial \bar{z}_k).$$

The overlaps of the symmetrized and the antisymmetrized states are different and hence the C-matrices and the Poisson brackets too. We compute

$$(C^s(z, \bar{z}))_{kl} = \delta_{kl} \tanh(z\bar{z}) - \bar{z}_k z_l / \cosh^2(z\bar{z})$$

and

$$(C^a(z, \bar{z}))_{kl} = \delta_{kl} \coth(z\bar{z}) - \bar{z}_k z_l / \sinh^2(z\bar{z}),$$

wich we have to invert to get the equations of motion. We will not mark the different Poisson brackets by extra signs; which one is meant will be clear from the functions inside.

1.7 Proposition:

1. The two functions $\mathfrak{H}^s$ and $\mathfrak{H}^a$ are invariant under permutation of the two particles

$$\mathfrak{H}^s(-z, -\bar{z}) = \mathfrak{H}^s(z, \bar{z}) \text{ and } \mathfrak{H}^a(-z, -\bar{z}) = \mathfrak{H}^a(z, \bar{z}).$$

2. If $z(t)$ is a solution of the e quations of motion given in the proposition above, the same holds true for $-z(t)$.

Proof:

1. Permutation of the particles changes z to $-z$. $|e_z^s\rangle$ is obviously invariant under this transformation and hence $\mathfrak{H}^s(z, \bar{z})$ too. In the antisymmetric case we have $|e_{-z}^a\rangle = -|e_z^a\rangle$. Therefore

$$\mathfrak{H}^a(-z, -\bar{z}) = \langle e_{-z}^a | H | e_{-z}^a\rangle / \langle e_{-z}^a | e_{-z}^a\rangle = \mathfrak{H}^a(z, \bar{z}),$$

because the additional minus signs cancel.

2. We can omit the superscripts and consider the two cases together. We find

$$(\partial \mathfrak{H}/\partial(-\bar{z}_k))(-z,-\bar{z}) = (\partial \mathfrak{H}/\partial \bar{z}_k)(z,\bar{z})$$

and

$$C^{-1}(-z,-\bar{z}) = C^{-1}(z,\bar{z}).$$

Replacing z by $-z$ in the equations of motion gives

$$-\dot{z}_l = i \sum_{k=1}^{3} (C^{-1}(-z,-\bar{z}))_{kl}(\partial \mathfrak{H}/\partial(-\bar{z}_k))(-z,-\bar{z})$$

which yields

$$-\dot{z}_l = i \sum_{k=1}^{3} (C^{-1}(z,\bar{z}))_{kl}(\partial \mathfrak{H}/\partial \bar{z}_k)(z,\bar{z}).$$

1.8 Proposition:

1. For symmetric and antisymmetric dequantization the classical functions for the creation operators Z_j vanish.
2. For quadratic combinations of the type $Z_j Z_k$ the classical functions are

$$(\mathfrak{Z}_j^s \circ \mathfrak{Z}_k^s)(z,\bar{z}) = z_j z_k \quad \text{or} \quad (\mathfrak{Z}_j^a \circ \mathfrak{Z}_k^a)(z,\bar{z}) = z_j z_k .$$

Proof:

One has to evaluate the expectation values.

1.9 Proposition:

The scalar product of the solutions of the equations of motion with themselves gives the classical function for ZZ.

$$(\mathfrak{Z}^s \circ \mathfrak{Z}^s)(t) = z(t)\, z(t) \quad \text{and} \quad (\mathfrak{Z}^a \circ \mathfrak{Z}^a)(t) = z(t)\, z(t).$$

Proof:

Follows from proposition 1.8.2.

The results of propositions 1.6–1.9 may be interpreted as follows: The classical equations of motion are invariant under permutation of particles and hence admit as solutions pairs of trajectories which are related by a permutation operation in classical phase space. In case of a closed trajectory, the permutation operation connects points on the same trajectory. The points on these trajectories do not determine the time-dependent expectation values of the relative position and momentum operators since these expectation values vanish, but they do determine the time-dependent expectation values of expressions quadratic in the position and momentum operators.

1.10 Examples:

1. Free particle in three dimensions

a) Kinetic energy for dequantization with coherent states: $\mathfrak{T}^c(z,\bar{z})/\hbar\omega = -(z-\bar{z})^2/4 + 3/4$.

b) Symmetric dequantization

$$\mathfrak{T}^s(z,\bar{z})/\hbar\omega = -(z-\bar{z})^2/4 + 3/4 - z\bar{z}/(1+\exp(2z\bar{z})).$$

The corresponding function on phase space is

$$\mathfrak{t}^s(x,p,\hbar) = p^2/2m + 3\hbar\omega/4 - ((x^2/b^2 + p^2 b^2/\hbar^2)/2)/(1+\exp(x^2/b^2 + p^2 b^2/\hbar^2)).$$

c) Antisymmetric dequantization

$$\mathfrak{T}^a(z,\bar{z})/\hbar\omega = -(z-\bar{z})^2/4 + 3/4 - z\bar{z}/(1-\exp(2z\bar{z})).$$

2. Gaussian interaction $V = \exp(-\gamma X^2/2)$.

a) Dequantization with coherent states

$$\mathfrak{V}^c(z,\bar{z}) = (1-4\mu)^{3/2} \exp(-2\mu(z+\bar{z})^2).$$

b) Symmetric dequantization

$$\mathfrak{V}^s(z,\bar{z}) = \mathfrak{V}^c(z,\bar{z})(1+\exp((8\mu-2)z\bar{z}))/(1+\exp(-2z\bar{z})).$$

c) Antisymmetric dequantization

$$\mathfrak{V}^a(z,\bar{z}) = \mathfrak{V}^c(z,\bar{z})(1-\exp((8\mu-2)z\bar{z}))/(1-\exp(-2z\bar{z})).$$

As we will later deal with different μ-parameters we will then refer to these interaction functions as $\mathfrak{V}^c(z,\bar{z},\mu)$, $\mathfrak{V}^s(z,\bar{z},\mu)$ and $\mathfrak{V}^a(z,\bar{z},\mu)$ respectively. μ has been introduced for convenience and contains the range parameter $\mu = \gamma b^2/(8+4\gamma b^2)$.

2. Dequantization of a Two-Nucleon System with an Effective Interaction

We study as a concrete example the relative motion of two nucleons with an effective interaction given by Arickx et al. [3]. This interaction is a sum of four Gaussians and splits into an attractive part

V_1 and a repulsive one V_2.

$$V_{\text{eff}} = V_1(X) + V_2(X), \quad \text{where}$$
$$V_i(X) = (\alpha_i^e P^e + \alpha_i^o P^o) \exp(-\gamma X^2/2).$$

P^e projects on even, P^o on odd states.

The following table shows the values of these parameters and of μ for particles without spin and isospin. The oscillator parameter is choosen $b = 1.6$ fm.

i	γ_i/fm	$\alpha_i^e/\hbar\omega$	$\alpha_i^o/\hbar\omega$	μ_i
1	4	− 23.92	− 5.09	0.20915
2	9	46.53	46.36	0.230032

Using example 1.10 we dequantize the Hamiltonian of the relative motion $H = P^2/2m + V_{\text{eff}}$. The expressions for the classical functions are valid for the three-dimensional case with $z \in \mathbb{C}^3$. We consider here a one-dimensional model, setting $z \in \mathbb{C}$, but maintain the zero-point oscillator energy and take the dimension-dependent exponent in the interaction function for $n = 3$.

2.1 Proposition:

With the notations of example 1.10 the classical functions for the Hamiltonian of the two-nucleon system are

a) for dequantization with coherent states

$$\mathfrak{H}^c(z,\bar z) = \mathfrak{T}^c(z,\bar z) + \sum_{i=1}^{2} \mathfrak{V}^c(z,\bar z,\mu_i) \cdot (\alpha_i^e + \alpha_i^o + (\alpha_i^e - \alpha_i^o) \exp((8\mu_i - 2) z\bar z))/2.$$

b) for symmetric dequantization

$$\mathfrak{H}^s(z,\bar z) = \mathfrak{T}^s(z,\bar z) + \sum_{i=1}^{2} \alpha_i^e \mathfrak{V}^s(z,\bar z,\mu_i).$$

c) for antisymmetric dequantization

$$\mathfrak{H}^a(z,\bar z) = \mathfrak{T}^a(z,\bar z) + \sum_{i=1}^{2} \alpha_i^o \mathfrak{V}^a(z,\bar z,\mu_i).$$

For each of the three corresponding functions on phase space $\mathfrak{h}^c$, $\mathfrak{h}^s$ and $\mathfrak{h}^a$ we can now plot the lines of constant energy.

Compared with $\mathfrak{h}^c$ (Fig. 1) the energy surface of $\mathfrak{h}^s$ (Fig. 2) is broader, which means stronger attrac-

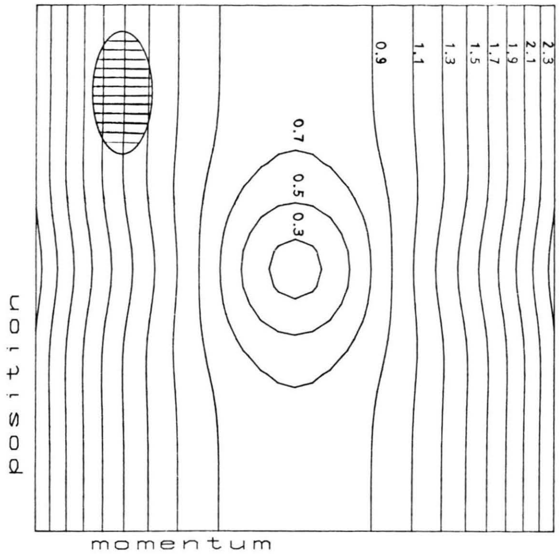

Fig. 1. Lines of constant energy for dequantization with coherent states, energy in units of $\hbar\omega$, in a section of phase space from $p = -6b/\hbar$ to $6b/\hbar$ and $x = -3\,b$ to $3b$. The ellipse indicates the size of the coherent state, the lengths of the half-axes are choosen as the root-mean-square deviations Δx and Δp respectively.

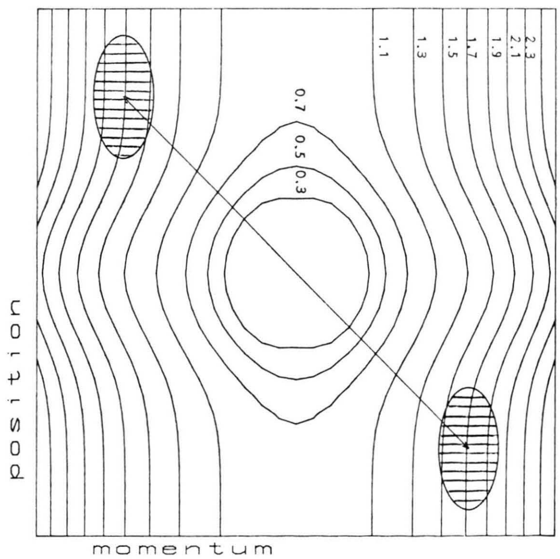

Fig. 2. Lines of constant energy for dequantization with symmetrized coherent states. The two ellipses show a corresponding pair of coherent states.

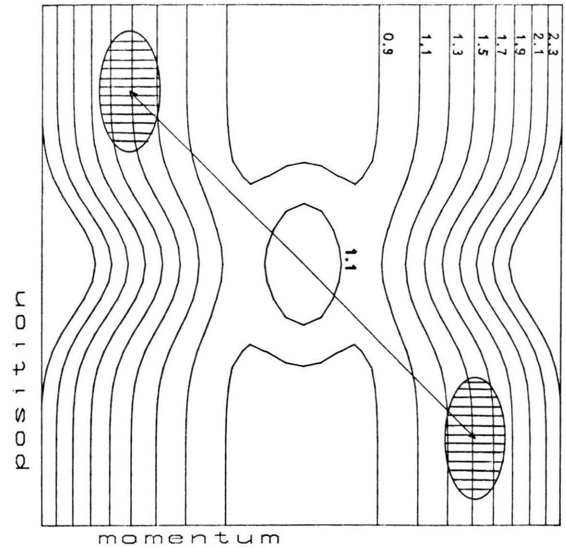

Fig. 3. Lines of constant energy for dequantization with antisymmetrized coherent states.

tion, whereas $\mathfrak{h}^a$ (Fig. 3) shows a significant additional repulsion. In the symmetric and the antisymmetric case there are nonlocal contributions to the energy, which can already be seen in the analytic expressions. In the outer regions all three plots converge to the free particle energy.

2.2 Proposition:

The energy at the origin of phase space is given through the matrix elements of H in the oscillator basis $\langle \tilde{N}\tilde{L}\tilde{M} | H | NLM \rangle$.

a) $\mathfrak{h}^c(0, 0, \hbar) = \langle 000 | H | 000 \rangle$

b) $\mathfrak{h}^s(0, 0, \hbar) = \langle 000 | H | 000 \rangle$

c) $\mathfrak{h}^a(0, 0, \hbar) = \langle 11M | H | 11M \rangle$.

Proof:

Expanding the coherent states with respect to the oscillator basis

$$|e_z\rangle = \sum_{NLM} |NLM\rangle \, P^N_{LM}(\bar{z}),$$

where the P^N_{LM} are the normalized states of a single particle with angular momentum in Bargmann space,

$$P^N_{LM}(z) = A_{NL}(z z)^{(N-L)/2} \, \mathfrak{Y}_{LM}(z),$$

$\mathfrak{Y}_{LM}$ is a solid spherical harmonic and

$$A_{NL} = (-1)^{(N-L)/2}(4\pi/(N+L+1)!!\,(N-L)!!)^{1/2}.$$

Considering

$$\langle e_{\bar{z}} | H | e_z \rangle = \sum_{\tilde{N}\tilde{L}\tilde{M}} \sum_{NLM} P^{\tilde{N}}_{\tilde{L}\tilde{M}}(\bar{z}) \cdot \langle \tilde{N}\tilde{L}\tilde{M} | H | NLM \rangle \, P^N_{LM}(z)$$

or $\langle e^s_{\bar{z}} | H | e^s_z \rangle$ and $\langle e^a_{\bar{z}} | H | e^a_z \rangle$ respectively for $z \to 0$ and $\bar{z} \to 0$ leads to the result.

2.3 Proposition:

Computing these values directly from the classical functions yields

a) $\mathfrak{h}^c(0, 0, \hbar) = 3\hbar\omega/4 + \sum_{i=1}^{2} \alpha^e_i (1 - 4\mu_i)^{3/2}$
$= -3.57$ MeV;

b) $\mathfrak{h}^s(0, 0, \hbar) = \mathfrak{h}^c(0, 0, \hbar)$;

c) $\mathfrak{h}^a(0, 0, \hbar) = 3\hbar\omega/4 + \hbar\omega/2 + \sum_{i=1}^{2} \alpha^o_i (1 - 4\mu_i)^{5/2}$
$= 20.72$ MeV.

The contribution due to the potential energy coincides with the matrix elements of the Arickx interaction.

$$\langle 000 | V_{\text{eff}} | 000 \rangle = -8.580 \text{ MeV},$$
$$\langle 11M | V_{\text{eff}} | 11M \rangle = 0.465 \text{ MeV}.$$

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[2] P. Kramer and M. Saraceno, Geometry of the Time-dependent Variational Principle in Quantum Mechanics, in: Springer Lecture Notes in Physics, Vol. **140,** Springer, Berlin 1981.
[3] F. Arickx, P. van Leuven, and M. Bouten, Z. Physik A **273,** 205 (1975).