Generating Function and a Rodrigues Formula for the Polynomials in $d$–Dimensional Semiclassical Wave Packets

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Abstract

We present a simple formula for the generating function for the polynomials in the $d$–dimensional semiclassical wave packets. We then use this formula to prove the associated Rodrigues formula.

1 Introduction

The generating function for 1–dimensional semiclassical wave packets is presented in formula (2.47) of [2]. In this paper, we present and prove the $d$–dimensional analog. As an application of this formula, we also prove the associated (multi–dimensional) Rodrigues formula.

These results have also been proven from a completely different point of view by Helge Dietert, Johannes Keller, and Stephanie Troppmann. See Lemma 3 and Section 3 (particularly Proposition 16) and formula (13) of [1]. See also [3]. We have also received a conjecture

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from Tomoki Ohsawa [4] that the generating function result could be proved abstractly by using the formula for products of Hermite polynomials and the action of the metaplectic group.

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## 2 Semiclassical Wave Packets

The semiclassical wave packets depend on two invertible $d \times d$ complex matrices $A$ and $B$ that are always assumed to satisfy

$$A^* B + B^* A = 2I \quad \text{and} \quad A^t B - B^t A = 0.$$ 

They also depend on a phase space point $(a, \eta)$ that plays no role in the present work. After choosing a branch of the square root, we define

$$\varphi_0(A, B, \hbar, a, \eta, x) = \pi^{-d/4} \hbar^{-d/4} (\det A)^{-1/2} \times \exp \left( - \frac{\langle (x-a), BA^{-1}(x-a) \rangle}{2\hbar} + i \frac{\langle \eta, (x-a) \rangle}{\hbar} \right).$$

Here, and for the rest of this paper, we regard $\mathbb{R}^d$ as being embedded in $\mathbb{C}^d$, and for any two vectors $a \in \mathbb{C}^d$ and $b \in \mathbb{C}^d$, we use the notation

$$\langle a, b \rangle = \sum_{j=1}^d \overline{a_j} b_j.$$

For $1 \leq l \leq d$, we define the $l$th raising operator

$$\mathcal{R}_l = \mathcal{A}_l(A, B, \hbar, a, \eta)^* = \frac{1}{\sqrt{2\hbar}} \left( \langle Be_l, (x-a) \rangle - i \langle A e_l, (-i\hbar \nabla - \eta) \rangle \right).$$

Then recursively, for any multi-index $k$, we define

$$\varphi_{k+e_l}(A, B, \hbar, a, \eta, x) = \frac{1}{\sqrt{k_l+1}} \mathcal{R}_l(\varphi_k(A, B, \hbar, a, \eta))(x).$$
For fixed $A$, $B$, $\hbar$, $a$, $\eta$, these wave packets form an orthonormal basis indexed by $k$. It is easy to see that

$$\varphi_k(A, B, \hbar, a, \eta, x) = 2^{-|k|/2} (k!)^{-1/2} P_k(A, \hbar, (x-a)) \varphi_0(A, B, \hbar, a, \eta, x),$$

where $P_k(A, \hbar, (x-a))$ is a polynomial of degree $|k|$ in $(x-a)$, although from this definition, it is not immediately obvious that $P_k(A, \hbar, (x-a))$ is independent of $B$.

Since they play no interesting role in what we are doing here, we henceforth assume $a = 0$ and $\eta = 0$.

3 The Generating Function

Our main result for the generating function is the following:

**Theorem 3.1** The generating function for the family of polynomials $P_k(A, \hbar, x)$ is

$$G(x, z) = \exp \left( -\langle z, A^{-1} x \rangle + \frac{2}{\sqrt{\hbar}} \langle z, A^{-1} x \rangle \right).$$

I.e.,

$$G(x, z) = \sum_k P_k(A, \hbar, x) \frac{z^k}{k!}.$$ 

**Remark** We make the unconventional definition $|A| = \sqrt{AA^*}$. By our conditions on the matrices $A$ and $B$, this forces $|A|$ to be real symmetric and strictly positive. We also have the polar decomposition $A = |A| U_A$, where $U_A$ is unitary. With this notation, we can write

$$G(x, z) = \exp \left( -\langle U_A z, U_A A^{-1} z \rangle + \frac{2}{\sqrt{\hbar}} \langle U_A z, |A|^{-1} x \rangle \right).$$

This equivalent formula is the one we shall actually prove.

We begin the proof of Theorem 3.1 with a lemma that provides an alternative formula for $R_l$. From this formula and an induction on $|k|$, one can easily prove that $P_k(A, \hbar, x)$ is independent of $B$, because

$$\overline{\varphi_0(A, B, \hbar, 0, 0, x)} \varphi_0(A, B, \hbar, 0, 0, x) = \pi^{-d/2} \hbar^{-d/2} |\det A|^{-1} \exp \left( -\frac{\langle x, \overline{|A|^{-2}} x \rangle}{\hbar} \right).$$
Lemma 3.2 For any $\psi \in S$,

$$ (R_l \psi)(x) = - \sqrt{\frac{\hbar}{2}} \frac{1}{\varphi_0(A, B, \hbar, 0, x)} \left\langle A e_l, \nabla \left( \varphi_0(A, B, \hbar, 0, x) \psi(x) \right) \right\rangle. $$

Proof: The gradient on the right hand side of the equation in the lemma can act either on the $\varphi_0$ or on the $\psi$. So, we get two terms when we compute this:

$$ \sqrt{\frac{\hbar}{2}} \left( \frac{1}{2 \hbar} \sum_{j=1}^{d} \left\langle A e_l, \left( e_j \left( \langle e_j, B A^{-1} x \rangle + \langle x, B A^{-1} e_j \rangle \right) \right) \psi(x) \right\rangle \right. $$

$$ \left. - \left\langle A e_l, \left( \nabla \psi \right)(x) \right\rangle \right). $$

The second term here is precisely the second term $\frac{1}{\sqrt{2} \hbar} (-i \langle A e_l, (-i \hbar \nabla) \psi(x) \rangle)$, in the expression for $(R_l \psi)(x)$. So, we need only show the first term here equals the first term, $\frac{1}{\sqrt{2} \hbar} \langle B e_l, x \rangle \psi(x)$, in the expression for $(R_l \psi)(x)$.

To do this, we begin by noting that the first term here equals

$$ \frac{1}{2 \sqrt{2} \hbar} \sum_{j=1}^{d} \left\langle A e_l, \left( e_j \left( \langle e_j, B A^{-1} x \rangle + \langle x, B A^{-1} e_j \rangle \right) \right) \psi(x) \right\rangle. $$

$$ = \frac{1}{2 \sqrt{2} \hbar} \sum_{j=1}^{d} \left\langle A e_l, \left( e_j \left( \langle e_j, B A^{-1} x \rangle + \langle B A^{-1} e_j, x \rangle \right) \right) \psi(x) \right\rangle. $$

$$ = \frac{1}{2 \sqrt{2} \hbar} \sum_{j=1}^{d} \left\langle A e_l, \left( e_j \left( \langle e_j, B A^{-1} x \rangle + \langle B A^{-1} e_j, x \rangle \right) \right) \psi(x) \right\rangle. $$

$$ = \frac{1}{2 \sqrt{2} \hbar} \sum_{j=1}^{d} \left\langle A e_l, \left( e_j \left( \langle e_j, B A^{-1} x \rangle + \langle e_j, (A^{-1})^* B^* x \rangle \right) \right) \psi(x) \right\rangle. $$

$$ = \frac{1}{\sqrt{2} \hbar} \left\langle A e_l, \frac{B A^{-1} + (A^{-1})^* B^*}{2} x \right\rangle \psi(x). $$

Because of the relations satisfied by $A$ and $B$, $B A^{-1}$ is (real symmetric) + $i$ (real symmetric). So, its conjugate, $\overline{B A}^{-1}$ has this same form. Thus, $\overline{B A}^{-1}$ equals its transpose, which
is \((A^{-1})^* B^*\). So, the quantity of interest here equals

\[
\frac{1}{\sqrt{2\hbar}} \langle Ae_l, (A^{-1})^* B^* x \rangle \psi(x)
\]

\[
= \frac{1}{\sqrt{2\hbar}} \langle e_l, A^* (A^{-1})^* B^* x \rangle \psi(x)
\]

\[
= \frac{1}{\sqrt{2\hbar}} \langle e_l, B^* x \rangle \psi(x)
\]

\[
= \frac{1}{\sqrt{2\hbar}} \langle Be_l, x \rangle \psi(x),
\]

which is what we had to show. 

**Proof of Theorem 3.1:** By an induction on \(|k|\), we prove there is a \(|k|^\text{th}\) order polynomial \(p_k\) in \(d\) variables with the following properties:

- \(P_k(A, \hbar, x) = p_k(|A|^{-1} x/\sqrt{\hbar}).\)

- \(\left(\frac{\partial}{\partial z}\right)^k G(x, z) = p_k(|A|^{-1} x/\sqrt{\hbar} - \overline{U_A} z) G(x, z).\)

The result then follows by setting \(z = 0\). We never compute the polynomial \(p_k\) because it may be complicated. We also use the notation \(p_k(A, \hbar, x) = p_k((|A|^{-1} x/\sqrt{\hbar}).\)

We define \(p_0 = 1\). Below, we inductively compute \(\left(\frac{\partial}{\partial z}\right)^{k+e_l} G(x, z)\). For our second condition above to hold, \(p_{k+e_l}\) must be defined via the sum of formulas (3.1) and (3.2). This uniquely defines the polynomial \(p_{k+e_l}\).

For \(k = 0\), the result is trivial since \(P_0(A, \hbar, x) = 1\).

For the induction step, it is sufficient to do the following for an arbitrary positive integer \(l \leq d:\)

**Assuming we have already proved these for some \(k\), we prove them for the multi–index \(k + e_l\).**

To do this, we begin by noting that

\[
\varphi_k(A, B, \hbar, 0, 0, x) = \frac{1}{\sqrt{k!}} R^k(\varphi_0(A, B, \hbar, 0, 0))(x).
\]
Also,
\[ \varphi_k(A, B, \hbar, 0, 0, x) = 2^{-|k|/2} (k!)^{-1/2} P_k(A, \hbar, x) \varphi_0(A, B, \hbar, 0, 0, x). \]

So,
\[ \mathcal{R}^k(\varphi_0(A, B, \hbar, 0, 0))(x) = 2^{-|k|/2} P_k(A, \hbar, x) \varphi_0(A, B, \hbar, 0, 0, x). \]

Thus, when we apply the \( l \)th raising operator, the polynomial \( P_k(A, \hbar, x) \) gets changed to
\[ \frac{1}{\sqrt{2}} P_{k+e_l}(A, \hbar, x). \]

Assuming the induction hypothesis, when we differentiate \( \frac{\partial^k G}{\partial z^k} \) with respect to \( z_l \), the \( z_l \) derivative can act on the \( G(x, z) \) or it can act on the \( p_k(|A|^{-1} x/\sqrt{\hbar} - \overline{U_A} z) \). When it acts on the \( G(x, z) \), we obtain
\[ 2 \left\langle U_A e_l, \left( |A|^{-1} x/\sqrt{\hbar} - \overline{U_A} z \right) \right\rangle p_k(|A|^{-1} x/\sqrt{\hbar} - \overline{U_A} z) G(x, z). \] (3.1)

From the induction hypotheses, this is a polynomial of degree \( |k| + 1 \) evaluated at the argument \( |A|^{-1} x/\sqrt{\hbar} - \overline{U_A} z \). Note that this result depends on the following calculation, with \( G(x, z) \) written with the polar decomposition of \( A \):

\[ \frac{\partial G}{\partial z_l}(x, z) = \left( - \left\langle U_A e_l, \overline{U_A} z \right\rangle - \left\langle U_A \overline{z}, U_A e_l \right\rangle + \frac{2}{\sqrt{\hbar}} \left\langle U_A e_l, |A|^{-1} x \right\rangle \right) G(x, z) \]
\[ = 2 \left\langle U_A e_l, \left( |A|^{-1} x/\sqrt{\hbar} - \overline{U_A} z \right) \right\rangle G(x, z). \]

When the \( \frac{\partial}{\partial z_l} \) acts on the polynomial, we either get zero or a polynomial of degree \( |k| - 1 \).
\[ - \left\langle (\nabla p_k)(|A|^{-1} x/\sqrt{\hbar} - \overline{U_A} z), \overline{U_A} e_l \right\rangle G(x, z) \]
\[ = - \left\langle U_A e_l, (\nabla p_k)(|A|^{-1} x/\sqrt{\hbar} - \overline{U_A} z) \right\rangle G(x, z). \] (3.2)

Recall that
\[ (R_l \psi)(x) = - \sqrt{\frac{\hbar}{2}} \frac{1}{\varphi_0(A, B, \hbar, 0, 0, x)} \left\langle A e_l, \nabla \left( \varphi_0(A, B, \hbar, 0, 0, x) \psi(x) \right) \right\rangle, \]
and that from our induction hypothesis,

\[
\phi_0(A, B, h, 0, 0, x) \phi_k(A, B, h, 0, 0, x)
\]

\[
= \pi^{-d/2} h^{-d/2} 2^{-k|/2} (k!)^{-1/2} \left| \det A \right|^{-1} p_k(A, h, x) \exp \left\{ - \frac{\langle x, |A|^{-2} x \rangle}{h} \right\}.
\]

When computing \( R_l \phi_k \) by this formula, the gradient in \( R_l \) can act on the exponential or the \( p_k(A, h, x) \). When it acts on the exponential, we get

\[
2^{-k|/2} (k!)^{-1/2} p_k(A, h, x) \sqrt{\frac{2}{h}} \langle A e_l, |A|^{-2} x \rangle \phi_0(A, B, h, 0, 0, x)
\]

\[
= 2^{-|k|+1/2} \sqrt{k_l + 1} ((k + e_l)!)^{-1/2} \\
	\times 2 \left\langle U_A e_l, |A|^{-1} x/\sqrt{h} \right\rangle p_k(A, h, x) \phi_0(A, B, h, 0, 0, x). \quad (3.3)
\]

When the gradient in \( R_l \) acts on the \( p_k(A, h, x) \), in \( R_l \phi_k \), we get the term

\[
- \sqrt{\frac{h}{2}} 2^{-k|/2} (k!)^{-1/2} \left\langle A e_l, \nabla_x (p_k(A, h, x)) \right\rangle \phi_0(A, B, h, 0, 0, x)
\]

\[
= -2^{-|k|+1/2} (k!)^{-1/2} \left\langle A e_l, \sum_{j=1}^{d} \langle e_j, (\nabla p_k)(A, h, x) \rangle |A|^{-1} e_j \right\rangle \phi_0(A, B, h, 0, 0, x)
\]

\[
= -2^{-|k|+1/2} (k!)^{-1/2} \left\langle A e_l, |A|^{-1} (\nabla p_k)(A, h, x) \right\rangle \phi_0(A, B, h, 0, 0, x)
\]

\[
= -2^{-|k|+1/2} \sqrt{k_l + 1} ((k + e_l)!)^{-1/2} \\
	\times \left\langle U_A e_l, (\nabla p_k)(A, h, x) \right\rangle \phi_0(A, B, h, 0, 0, x). \quad (3.4)
\]

From \( 3.1 \) and \( 3.2 \) with \( z = 0 \), we obtain

\[
2 \left\langle U_A e_l, |A|^{-1} x/\sqrt{h} \right\rangle p_k(A, h, x) - \left\langle U_A e_l, (\nabla p_k)(|A|^{-1} x/\sqrt{h}) \right\rangle.
\]

From \( 3.3 \) and \( 3.4 \) and taking into account the factor of \( \sqrt{k_l + 1} \) in \( R_l(\phi_k) = \sqrt{k_l + 1} \phi_{k+e_l} \), we obtain

\[
P_{k+e_l}(A, h, x)
\]

\[
= 2 \left\langle U_A e_l, |A|^{-1} x/\sqrt{h} \right\rangle p_k(A, h, x) - \left\langle U_A e_l, (\nabla p_k)(|A|^{-1} x/\sqrt{h}) \right\rangle.
\]
The quantities of interest contain the same polynomial evaluated at the appropriate arguments, and $P_{k+e_l}(A, h, x) = p_{k+e_l}(A, h, x)$. Since $l$ is arbitrary, with $1 \leq l \leq d$, the result is true for all multi-indices with order $|k| + 1$, and the induction can proceed.

4 The Rodrigues Formula

As an application of the Generating Function formula, we prove a multi–dimensional Rodrigues formula for these polynomials. The result is

**Theorem 4.1** In $d$–dimensions, with the convention that $|A|$ is the positive square root of $AA^*$,

$$P_k(A, h, x) = \exp \left( \frac{||A|^{-1}x||^2}{h} \right) \left(-\sqrt{h}A^* \nabla_x \right)^k \exp \left(-\frac{||A|^{-1}x||^2}{h} \right).$$

**Remark** By scaling, it is sufficient to prove this for $h = 1$.

We begin the proof of this result with a lemma that embodies a special case of the chain rule for high order derivatives in $d$–dimensions.

**Lemma 4.2** Assume $F : \mathbb{R}^d \to \mathbb{R}^d$ is $C^m$ and that $M : \mathbb{R}^d \to \mathbb{R}^d$ is linear. Then viewing gradients as column vectors and using multi–index notation,

$$(\nabla_x)^m F(Mx) = \left( (M^t \nabla_y)^m F \right)_{y=Mx}$$

One proves this by induction on $|m|$, proving that each component is correct.

**Proof of Theorem 4.1** Using this technical result and the generating function,

$$P_k(A, 1, x)$$

$$= (\nabla_z)^k \exp \left(- (\overline{U_A} z)^t (\overline{U_A} z) + 2 (\overline{U_A} z)^t (|A|^{-1} x) \right)_{z=0}$$

$$= (\nabla_z)^k \exp \left(- (\overline{U_A} z - |A|^{-1} x)^t (\overline{U_A} z - |A|^{-1} x) \right) \exp \left((|A|^{-1} x)^t (|A|^{-1} x) \right)_{z=0}$$

$$= \exp \left((|A|^{-1} x)^t (|A|^{-1} x) \right) (\nabla_z)^k \exp \left(- (\overline{U_A} z - |A|^{-1} x)^t (\overline{U_A} z - |A|^{-1} x) \right)_{z=0}$$

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\[
\begin{align*}
\exp((|A|^{-1}x)^t (|A|^{-1}x)) & \quad \left((\overline{U_A})^t \nabla w\right)^k \exp\left(-(w - |A|^{-1}x)^t (w - |A|^{-1}x)\right)_{w=0} \\
= \exp((|A|^{-1}x)^t (|A|^{-1}x)) & \quad \left((\overline{U_A})^t \nabla w\right)^k \exp\left(-(w - u)^t (w - u)\right)_{u = |A|^{-1}x} \\
= \exp((|A|^{-1}x)^t (|A|^{-1}x)) & \quad \left(- (\overline{U_A})^t \nabla u\right)^k \exp\left(-(w - u)^t (w - u)\right)_{u = |A|^{-1}x} \\
= \exp((|A|^{-1}x)^t (|A|^{-1}x)) & \quad \left(\overline{U_A})^t |A|^t \nabla x\right)^k \exp\left(-(w - |A|^{-1}x)^t (w - |A|^{-1}x)\right)_{w=0} \\
= \exp((|A|^{-1}x)^t (|A|^{-1}x)) & \quad \left(- (\overline{U_A})^t |A|^t \nabla x\right)^k \exp\left(- (|A|^{-1}x)^t (|A|^{-1}x)\right) \\
\end{align*}
\]

However, $|A|^t = |A|$ is real, and with our unusual convention, $A = |A| U_A$. So, $(\overline{U_A})^t |A| = A^*$. This proves the theorem.  

References

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