

Generating Functions 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.

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.

This result has also been proven from a different point of view by Helge Dietert, Johannes Keller, and Stephanie Troppmann. See Lemma 3 and Section 3 (particularly Proposition 16) of [1]. We have also received a conjecture from Tomoki Ohsawa [3] that this 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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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, η) that plays no role in the present work. After choosing a branch of the square root, we define

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

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

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

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

$$\mathcal{R}_l = \mathcal{A}_l(A, B, \hbar, 0, 0)^* = \frac{1}{\sqrt{2\hbar}} (\langle B e_l, (x-a) \rangle - i \langle A e_l, (-i\hbar\nabla - \eta) \rangle).$$

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, η , 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 $\eta = 0$.

Our main result is the following:

Theorem 1.1 *The generating function for the family of polynomials $P_k(A, \hbar, x)$ is*

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

I.e.,

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

Remark We make the unconventional definition $|A| = \sqrt{A A^*}$. 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

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

This equivalent formula is the one we shall actually prove.

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2 Proof of the Theorem

We begin with a lemma that provides an alternative formula for \mathcal{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

$$\overline{\varphi_0(A, B, \hbar, 0, 0, x)} \varphi_0(A, B, \hbar, 0, 0, x) = \pi^{-1/2} \hbar^{-1/2} |\det A|^{-1} \exp \left(- \frac{\langle x, |A|^{-2} x \rangle}{\hbar} \right).$$

Lemma 2.1 *For any $\psi \in \mathcal{S}$,*

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

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

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

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

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

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

$$\begin{aligned}
& \frac{1}{\sqrt{2\hbar}} \langle A e_l, (A^{-1})^* B^* x \rangle \psi(x) \\
&= \frac{1}{\sqrt{2\hbar}} \langle e_l, A^* (A^{-1})^* B^* x \rangle \psi(x) \\
&= \frac{1}{\sqrt{2\hbar}} \langle e_l, B^* x \rangle \psi(x) \\
&= \frac{1}{\sqrt{2\hbar}} \langle B e_l, x \rangle \psi(x),
\end{aligned}$$

which is what we had to show. ■

Proof of the Theorem: We prove the theorem by an induction on $|k|$. For $k = 0$, the result is trivial since $P_0(A, \hbar, x) = 1$.

Without ever computing an explicit formula for the polynomial p_k (which may be complicated), we prove inductively that

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

and

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

The result then follows by setting $z = 0$.

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

$$\varphi_k(A, B, \hbar, 0, 0, x) = \frac{1}{\sqrt{k!}} \mathcal{R}^k(\varphi_0(A, B, \hbar, 0, 0))(x).$$

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 $p_k(|A|^{-1} x / \sqrt{\hbar} - U_A z)$. When it acts on the $G(x, z)$, we obtain

$$2 \left\langle U_A e_l, \left(|A|^{-1} x / \sqrt{\hbar} - \overline{U_A} z \right) \right\rangle p_k(A, \hbar, x) G(x, z). \quad (2.1)$$

Note that this result depends on the following calculation, with $G(x, z)$ written with the polar decomposition of A :

$$\begin{aligned}
\frac{\partial G}{\partial z_k}(x, z) &= \left(-\langle U_A e_l, \overline{U_A z} \rangle - \langle U_A \bar{z}, \overline{U_A e_l} \rangle + \frac{2}{\sqrt{\hbar}} \langle U_A e_l, |A|^{-1} x \rangle \right) G(x, z) \\
&= 2 \left\langle U_A e_l, \left(|A|^{-1} x / \sqrt{\hbar} - \overline{U_A z} \right) \right\rangle G(x, z).
\end{aligned}$$

When the $\frac{\partial}{\partial z_l}$ acts on the polynomial, we get

$$\begin{aligned}
&- \left\langle \overline{(\nabla p_k)(|A|^{-1} x / \sqrt{\hbar} - \overline{U_A z})}, \overline{U_A e_l} \right\rangle G(x, z) \\
&= - \left\langle U_A e_l, (\nabla p_k)(|A|^{-1} x / \sqrt{\hbar} - \overline{U_A z}) \right\rangle G(x, z). \tag{2.2}
\end{aligned}$$

Recall that

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

and that from our induction hypothesis,

$$\overline{\varphi_0(A, B, \hbar, 0, 0, x)} \varphi_k(A, B, \hbar, 0, 0, x) = 2^{-|k|/2} (k!)^{-1/2} p_k(A, \hbar, x) e^{-\frac{\langle x, |A|^{-2} x \rangle}{\hbar}}.$$

The gradient in \mathcal{R}_l can act on the exponential or the $p_k(A, \hbar, x)$. When it acts on the exponential, we get

$$\begin{aligned}
&2^{-|k|/2} (k!)^{-1/2} p_k(A, \hbar, x) \sqrt{\frac{2}{\hbar}} \left\langle A e_l, |A|^{-2} x \right\rangle \varphi_0(A, B, \hbar, 0, 0, x) \\
&= 2^{-(|k|+1)/2} \sqrt{k_l + 1} ((k + e_l)!)^{-1/2} \\
&\quad \times 2 \left\langle U_A e_l, |A|^{-1} x / \sqrt{\hbar} \right\rangle p_k(A, \hbar, x) \varphi_0(A, B, \hbar, 0, 0, x). \tag{2.3}
\end{aligned}$$

When the gradient in \mathcal{R}_l acts on the $p_k(A, \hbar, x)$, we get

$$\begin{aligned}
&- \sqrt{\frac{\hbar}{2}} 2^{-|k|/2} (k!)^{-1/2} \left\langle A e_l, \nabla_x p_k(A, \hbar, x) \right\rangle \varphi_0(A, B, \hbar, 0, 0, x) \\
&= - 2^{-(|k|+1)/2} (k!)^{-1/2} \left\langle A e_l, \sum_{j=1}^d \langle e_j, (\nabla p_k)(A, \hbar, x) \rangle |A|^{-1} e_j \right\rangle \varphi_0(A, B, \hbar, 0, 0, x)
\end{aligned}$$

$$\begin{aligned}
&= - 2^{-(|k|+1)/2} (k!)^{-1/2} \langle A e_l, |A|^{-1} (\nabla p_k)(A, \hbar, x) \rangle \varphi_0(A, B, \hbar, 0, 0, x) \\
&= - 2^{-(|k|+1)/2} \sqrt{k_l + 1} ((k + e_l)!)^{-1/2} \\
&\quad \times \langle U_A e_l, (\nabla p_k)(A, \hbar, x) \rangle \varphi_0(A, B, \hbar, 0, 0, x). \tag{2.4}
\end{aligned}$$

From (2.1) and (2.2) with $z = 0$, we obtain

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

From (2.3) and (2.4) and taking into account the factor of $\sqrt{k_l + 1}$ in $\mathcal{R}_l(\varphi_k) = \sqrt{k_l + 1} \varphi_{k+e_l}$, we obtain

$$\begin{aligned}
&P_{k+e_l}(A, \hbar, x) \\
&= 2 \left\langle U_A e_l, |A|^{-1} x / \sqrt{\hbar} \right\rangle p_k(A, \hbar, x) - \left\langle U_A e_l, (\nabla p_k)(|A|^{-1} x / \sqrt{\hbar}) \right\rangle.
\end{aligned}$$

The quantities of interest contain the same polynomial evaluated at the appropriate arguments, and $P_{k+e_l}(A, \hbar, x) = p_{k+e_l}(A, \hbar, x)$. 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. ■

References

- [1] Dietert, H., Keller, J., and Troppmann, S.: An Invariant Class of Hermite Type Multivariate Polynomials for the Wigner Transform. (2015 preprint, arXiv:1505.06192).
- [2] Hagedorn, G.A.: Raising and Lowering Operators for Semiclassical Wave Packets. *Ann. Phys.* **269**, 77–104 (1998).
- [3] Ohsawa, T.: private communication.