Generating Functions for the Polynomials in $d$–Dimensional Semiclassical Wave Packets

George A. Hagedorn*
Department of Mathematics and
Center for Statistical Mechanics and Mathematical Physics
Virginia Polytechnic Institute and State University
Blacksburg, Virginia 24061-0123, U.S.A.

May 24, 2015

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.

*Partially Supported by National Science Foundation Grant DMS–1210982.
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

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

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

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

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

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

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

\[ \varphi_{k+l}(A, B, \hbar, a, \eta, x) = \frac{1}{\sqrt{k_l + 1}} \mathcal{R}_l(\varphi_k(A, B, \hbar, a, \eta))(x). \]

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 $\eta = 0$.

Our main result is the following:
Theorem 1.1 The generating function for the family of polynomials \( P_k(A, \hbar, x) \) is
\[
G(x, z) = \exp \left( - \left\langle z, A^{-1} A z \right\rangle + \frac{2}{\sqrt{\hbar}} \left\langle z, A^{-1} x \right\rangle \right).
\]
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
\[
G(x, z) = \exp \left( - \left\langle U_A z, U_A z \right\rangle + \frac{2}{\sqrt{\hbar}} \left\langle U_A z, |A|^{-1} x \right\rangle \right).
\]
This equivalent formula is the one we shall actually prove.

Acknowledgements It is a pleasure to thank Raoul Bourquin and Vasile Gradinaru for motivating this work. It is also a pleasure to thank Johannes Keller, Tomoki Ohsawa, Sam Robinson, and Leonardo Mihalcea for their enthusiasm and numerous comments.

2 Proof of the Theorem

We begin with a lemma that provides an alternative formula for \( \mathcal{R}_t \). From this formula and an induction on \( |k| \), one can easily prove that \( P_k(A, \hbar, x) \) is independent of \( B \), because
\[
\varphi_0(A, B, \hbar, 0, 0, x) \varphi_0(A, B, \hbar, 0, 0, x) = \pi^{-1/2} \hbar^{-1/2} |\det A|^{-1} \exp \left( - \frac{\left\langle x, |A|^{-2} x \right\rangle}{\hbar} \right).
\]

Lemma 2.1 For any \( \psi \in \mathcal{S} \),
\[
(R_t \psi)(x) = - \sqrt{\frac{\hbar}{2}} \frac{1}{\varphi_0(A, B, \hbar, 0, 0, x)} \left\langle A e_l, \nabla \left( \varphi_0(A, B, \hbar, 0, 0, x) \psi(x) \right) \right\rangle.
\]

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:
\[
\sqrt{\frac{\hbar}{2}} \left( \frac{1}{2 \hbar} \sum_{j=1}^d \left\langle A e_l, \left( e_j \left\langle e_j, B A^{-1} x \right\rangle + \left\langle x, B A^{-1} e_j \right\rangle \right) \right\rangle \psi(x)
- \left\langle A e_l, \left( \nabla \psi(x) \right) \right\rangle \right).
\]
The second term here is precisely the second term \( \frac{1}{\sqrt{2\hbar}} (-i \langle Ae_l, (-i \hbar \nabla) \psi(x) \rangle) \), in the expression for \((R_l \psi)(x)\). So, we need only show the first term here equals the first term, \( \frac{1}{\sqrt{2\hbar}} \langle Be_l, x \rangle \psi(x) \), in the expression for \((R_l \psi)(x)\).

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

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

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

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

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

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

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

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

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

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

\[
= \frac{1}{\sqrt{2\hbar}} \left( B e_l, x \right) \psi(x), 
\]

which is what we had to show. \( \blacksquare \)
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

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

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

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

Note that this result depends on the following calculation, with $G(x, z)$ written with the polar decomposition of $A$:
\[
\frac{\partial G}{\partial z_k}(x, z) = \left( - \langle U_A e_l, \overline{U}_A z \rangle - \langle U_A z, \overline{U}_A e_l \rangle + \frac{2}{\sqrt{\hbar}} \langle U_A e_l, |A|^{-1} x \rangle \right) G(x, z)
\]
\[
= 2 \left\langle U_A e_l, \left( |A|^{-1} x/\sqrt{\hbar} - \overline{U}_A z \right) \right\rangle G(x, z).
\]

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

\[
- \left\langle (\nabla p_k)(|A|^{-1} x/\sqrt{\hbar} - \overline{U}_A z), \overline{U}_A e_l \right\rangle G(x, z)
\]
\[
= - \left\langle U_A e_l, (\nabla p_k)(|A|^{-1} x/\sqrt{\hbar} - \overline{U}_A z) \right\rangle G(x, z).
\quad \text{(2.2)}
\]

Recall that

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

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

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

\[
2^{-|k|/2} (k!)^{-1/2} p_k(A, h, x) \sqrt{\frac{2}{\hbar}} \langle A e_l, |A|^{-2} x \rangle \varphi_0(A, B, h, 0, 0, x)
\]
\[
= 2^{-|k|/2} (k!)^{-1/2} \sqrt{k_l + 1} ((k + e_l)!)^{-1/2}
\]
\[
\times 2 \left\langle U_A e_l, |A|^{-1} x/\sqrt{\hbar} \right\rangle p_k(A, h, x) \varphi_0(A, B, h, 0, 0, x).
\quad \text{(2.3)}
\]

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

\[
- \sqrt{\frac{\hbar}{2}} 2^{-|k|/2} (k!)^{-1/2} \left\langle A e_l, \nabla_p e p_k(A, h, x) \right\rangle \varphi_0(A, B, h, 0, 0, x)
\]
\[
= - 2^{-|k|/2} (k!)^{-1/2} \left\langle A e_l, \sum_{j=1}^{d} (e_j, (\nabla p_k)(A, h, x)) |A|^{-1} e_j \right\rangle \varphi_0(A, B, h, 0, 0, x)
\]
\[
= -2^{-(|k|+1)/2}(k!)^{-1/2} \left\langle Ae_l, |A|^{-1}(\nabla p_k)(A, \hbar, x) \right\rangle \varphi_0(A, B, \hbar, 0, 0, x)
\]

\[
= -2^{-(|k|+1)/2}\sqrt{k_l + 1} \left((k + e_l)!ight)^{-1/2}
\]

\[
\times \left\langle U_Ae_l, (\nabla p_k)(A, \hbar, x) \right\rangle \varphi_0(A, B, \hbar, 0, 0, x).
\]  (2.4)

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

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

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

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

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

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. \(\blacksquare\)

References

