

Gaussian-Wigner distributions in quantum mechanics and optics

R. Simon and E. C. G. Sudarshan

The Institute of Mathematical Sciences, C.I.T. Campus, Madras 600 113, India

N. Mukunda

Centre for Theoretical Studies, Indian Institute of Science, Bangalore 560 012, India

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Gaussian kernels representing operators on the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^n)$ are studied. Necessary and sufficient conditions on such a kernel in order that the corresponding operator be positive semidefinite, corresponding to a density matrix (cross-spectral density) in quantum mechanics (optics), are derived. The Wigner distribution method is shown to be a convenient framework for characterizing Gaussian kernels and their unitary evolution under $Sp(2n, \mathbb{R})$ action. The nontrivial role played by a phase term in the kernel is brought out. The entire analysis is presented in a form which is directly applicable to n -dimensional oscillator systems in quantum mechanics and to Gaussian Schell-model partially coherent fields in optics.

I. INTRODUCTION

The Wigner distribution gives a description of states in quantum mechanics closely resembling the statistical phase-space description of classical systems, without, however, losing any of the specific features of quantum mechanics.¹ It works at the level of the density operator rather than the state vector, so the superposition principle of quantum mechanics is not manifest. It is related to the Weyl correspondence between classical and quantum-dynamical variables in a natural way.^{2,3}

In recent times a closely analogous method based on the so-called Wolf function has been introduced into statistical optics.⁴ This development is part of the relatively recent understanding of the relationships between radiative transfer and radiometry on the one hand, and electrodynamics and physical optics on the other,^{5,6} although the fact that the ray-optics-wave-optics connection is largely identical to the classical-mechanics-quantum-mechanics connection has been known for a long time. The basic objects such as specific intensity and radiance in radiative transfer and radiometry are formally analogous to the phase-space distribution in classical mechanics. The Wolf function⁴ is defined as a partial Fourier transform, or Moyal transform, of the two-point cross-spectral density of the optical field, just as the Wigner function is the Moyal transform of the configuration space density matrix in quantum mechanics. It tries to capture as many of the simple properties of rays in geometrical optics as possible, without sacrificing the specifically wave optical features of interference and diffraction; this is achieved through the introduction of the concept of generalized rays.⁴

The cross-spectral density in optics and the density matrix in quantum mechanics have very similar defining properties. In a configuration-space description, both can be viewed as operators on a Hilbert space $L^2(\mathbb{R}^n)$ of square integrable functions for suitable n , and both are Hermitian positive semidefinite. The only difference is

that, while in the optical case we require a finite trace, in quantum mechanics the trace must be unity corresponding to normalization of probability. As a consequence of this formal similarity, many of the well-known properties of the Wigner distribution pass over to corresponding properties of the Wolf function, with appropriate changes in interpretation.

Let us recall some of the more notable results concerning the Wigner distribution in quantum mechanics. It is well known that it is not a true phase-space probability distribution but only a "quasiprobability distribution," since for a general state it is not pointwise non-negative. In fact, the only pure states for which the Wigner distribution is everywhere non-negative are those for which the Schrödinger wave function is Gaussian.⁷ Although the Wigner distribution is thus in general indefinite, it turns out that the convolution of two Wigner distributions is always a non-negative function on phase space. This resulting function is in general, however, not a Wigner distribution corresponding to any state.⁸ Nevertheless, attempts have been made to interpret the convolution process as the coarse graining effected by the interaction between a quantum system and a measuring apparatus, the input Wigner distributions referring to system and apparatus, respectively.⁹ Another property of Wigner distributions is that they cannot be arbitrarily sharply peaked in phase space since they must after all reproduce the uncertainty relations.

The Wolf function has similar properties. It is a real function on the phase space appropriate for light, but for a general cross-spectral density it can take on both positive and negative values. Thus it can only be thought of as a quasi-intensity distribution of generalized rays of light. The only fully coherent optical fields for which the Wolf function is non-negative everywhere are those for which the field amplitude is Gaussian. The positive semidefiniteness of the associated Hilbert space operator is reflected in properties of the Wigner distribution and the Wolf function in identical ways. While the Wolf

function cannot also be arbitrarily sharply peaked in the space of its arguments, the convolution properties of Wigner distributions mentioned above do not have an established measurement theoretical meaning in the optical context.

The use of the Wolf function becomes practically convenient in paraxial propagation problems. In this case, the family of Gaussian Schell-model fields generated by partially coherent planar sources of a particular type have received particular attention. One speaks of isotropic¹⁰ or anisotropic¹¹ Gaussian Schell-model fields (IGSM or AGSM) according to whether or not there is invariance with respect to rotations about the beam axis. In the IGSM case the cross-spectral density in any transverse plane has the form¹²

$$\begin{aligned}\Gamma(\mathbf{q}; \mathbf{q}') = & A \exp[-\mathbf{q}^T L \mathbf{q} - \mathbf{q}'^T L \mathbf{q}' - \frac{1}{2}(\mathbf{q} - \mathbf{q}')^T M(\mathbf{q} - \mathbf{q}') \\ & + \frac{i}{2}(\mathbf{q} - \mathbf{q}')^T K(\mathbf{q} + \mathbf{q}')].\end{aligned}\quad (1.1)$$

Here \mathbf{q} and \mathbf{q}' are two-dimensional position vectors in the transverse plane, while L, M are real, L being positive and M non-negative, and K a real parameter. Clearly, L^{-1} , M^{-1} , and K are, respectively, measures of the intensity width, the coherence length, and the phase curvature. This three-parameter family of IGSM fields transforms into itself not only under free propagation but also under action by all axially symmetric first-order optical systems (FOS's).¹² In wave optics an FOS acts on the amplitude via the generalized Huyghens integral,¹³ which as is known furnishes a unitary representation of the group $\text{Sp}(2, \mathbb{R})$ on $L^2(\mathbb{R})$ (in the axially symmetric case). In the language of generalized rays, the same system acts on the ray parameters through the numerical $\text{Sp}(2, \mathbb{R})$ ray-transfer matrix. We have analyzed elsewhere the transformation of IGSM fields by FOS's, using the generalized ray distribution or Wolf function. For such fields, this function is again Gaussian, being determined by a 2×2 real, symmetric, positive definite parameter matrix G ; the positive semidefiniteness of the cross-spectral density (1.1) interpreted as an operator kernel leads to $\det G \leq 1$. Using the local isomorphisms $\text{Sp}(2, \mathbb{R}) = \text{SL}(2, \mathbb{R}) \simeq \text{SO}(2, 1)$, a geometrical picture has been developed in which IGSM fields and FOS's can be represented, respectively, as timelike vectors and Lorentz transformations in a fictitious $(2+1)$ -dimensional Minkowski space. This picture makes it particularly easy to visualize many of the properties of this class of fields. In particular, it leads to a natural generalization of Kogelnik's "abcd law"¹⁴ to the partially coherent IGSM beams.¹²

When rotational invariance about the beam axis is given up, L and M become 2×2 real symmetric matrices, L being positive definite and M positive semidefinite, while K is a real matrix. We then have the ten-parameter family of AGSM fields.¹⁵ One can also consider FOS's without axial symmetry, which make up the group $\text{Sp}(4, \mathbb{R})$;¹⁶ these now map the family of all AGSM fields onto itself. The (astigmatic) FOS acts by a unitary representation of $\text{Sp}(4, \mathbb{R})$ on $L^2(\mathbb{R}^2)$ in the wave-optic description, and by a numerical $\text{Sp}(4, \mathbb{R})$ ray-

transfer matrix in the generalized ray description. The Wolf function is Gaussian again but now characterized by a 4×4 real symmetric positive definite matrix G . Compared with the IGSM case, however, the implications on G of the positive semidefiniteness of the kernel (1.1) are much more intricate. We also succeeded in developing a geometrical picture based on the local isomorphism $\text{Sp}(4, \mathbb{R}) \simeq \text{SO}(3, 2)$. In this picture, each AGSM field is represented by an antisymmetric second-rank tensor, and each FOS by a de Sitter rotation, in a $(3+2)$ -dimensional space. This analysis showed that the possible AGSM fields are made up of two distinct families or types, corresponding to distinct kinds of orbits under the adjoint action in the Lie algebra of $\text{SO}(3, 2)$.¹⁵

As a converse to the process of transferring known results on Wigner distributions to new results for the Wolf function, we can also state the following: for every cross-spectral density allowed by general principles, there must exist a state of a suitable quantum-mechanical system such that the given cross-spectral density can be reinterpreted as the configuration-space density matrix of the state. In this sense, the family of IGSM cross-spectral densities becomes the density matrices of the thermal states of a one-dimensional harmonic oscillator, and their $\text{Sp}(2, \mathbb{R})$ transforms. A similar identification can be made for AGSM fields and states of a two-dimensional oscillator. For oscillators with N degrees of freedom we have to deal with the group $\text{Sp}(2n, \mathbb{R})$. Their thermal states and all $\text{Sp}(2n, \mathbb{R})$ transforms thereof, will have density matrices of the form (1.1) but with \mathbf{q} and \mathbf{q}' being n -component vectors, and L, M, K being suitable $n \times n$ matrices.

Following this generalization of the kernel (1.1) to n -dimensional vectors \mathbf{q}, \mathbf{q}' , we see that operators on $L^2(\mathbb{R}^n)$ with such kernels play an important role both in optics and in quantum mechanics. All such kernels lead, via the Moyal transform, to Gaussian phase-space distributions (Wolf or Wigner) characterized by a $2n$ -dimensional real parameter matrix G . Given the Gaussian kernel (1.1), it is important to know the conditions on the n -dimensional real matrices L, M , and K which will ensure that this kernel is a bona fide cross-spectral density or density matrix. In the phase-space version, it is important to characterize the necessary and sufficient conditions on G so that the Gaussian phase-space distribution will be an allowed Wolf or Wigner function.¹⁷ The present paper addresses itself to a complete analysis of these questions. We present the work in such a way as to make the results applicable in both contexts. A particularly delicate point which will be brought out is the role of the "phase matrix" K , which becomes evident only for $N \geq 2$ and which was not identified in Ref. 15 where we studied AGSM fields.

The contents of the paper are as follows. In Sec. II we derive some algebraic properties of the Moyal transform which give an essentially complete characterization of this transform. In particular, the unitary $\text{Sp}(2n, \mathbb{R})$ action on $L^2(\mathbb{R}^n)$ via an n -dimensional Huyghens integral appears extremely simple in terms of the Moyal transform, when one is considering operators on, rather than wave functions in, $L^2(\mathbb{R}^n)$. The problem of finding the

necessary and sufficient conditions for a Gaussian phase-space distribution to be a Wolf (Wigner) function is formulated and solved in Secs. III and IV. We use the fact that under the $Sp(2n, \mathbb{R})$ action the operator with the Gaussian kernel (1.1) undergoes a unitary similarity transformation which preserves the defining properties of a density operator or cross-spectral density. Hence the $Sp(2n, \mathbb{R})$ action can be used to take the associated Moyal transform to a standard or normal form where the defining properties can be conveniently tested. All this is made possible by a basic theorem of Williamson¹⁸ concerning normal forms of quadratic Hamiltonians. The complete set of necessary and sufficient conditions is presented explicitly in terms of certain $Sp(2n, \mathbb{R})$ invariants of the G matrix. In Sec. V. the important role of, and restrictions on, the phase matrix K which arise only for $N \geq 2$ are highlighted. This was missed in Ref. 15 and this incompleteness is rectified here. It turns out that only the antisymmetric part of K is subject to definite restrictions, which explains why there are no such conditions for IGSM fields. The final section, Sec. VI, contains some concluding remarks.

II. ALGEBRAIC PROPERTIES OF THE MOYAL TRANSFORM

We develop here some algebraic properties of the Wigner-Moyal transform, familiar from quantum mechanics, with respect to the real symplectic group $Sp(2n, \mathbb{R})$. These properties amount essentially to a complete characterization of this transform. Consider an irreducible set of Hermitian operators $\hat{q}_r, \hat{p}_r, r = 1, 2, \dots, n$ obeying the familiar canonical commutation relations

$$[\hat{q}_r, \hat{p}_s] = i\delta_{rs}, \quad [\hat{q}_r, \hat{q}_s] = [\hat{p}_r, \hat{p}_s] = 0. \quad (2.1)$$

The Schrödinger realization of these operators uses the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^n)$ of square integrable functions of n real variables $q_r, r = 1, 2, \dots, n$:

$$\mathcal{H} = \left\{ \psi(\mathbf{q}) \mid \int_{\mathbb{R}^n} d^n q |\psi(\mathbf{q})|^2 < \infty \right\}. \quad (2.2)$$

(The symbol \mathbf{q} , and similarly \mathbf{p} later on, stands for the n -tuple q_1, q_2, \dots, q_n .) On this space the \hat{q}_r act as operators of multiplication while the \hat{p}_r act as operators of differentiation; in the familiar notation using an ideal basis for \mathcal{H} made up of simultaneous eigenvectors $|\mathbf{q}\rangle$ of the \hat{q}_r , one has

$$\begin{aligned} \hat{q}_r |\mathbf{q}\rangle &= q_r |\mathbf{q}\rangle, \\ \langle \mathbf{q}' | \mathbf{q}\rangle &= \delta^{(n)}(\mathbf{q}' - \mathbf{q}), \quad -\infty < q_r < \infty, \\ \psi(\mathbf{q}) &= \langle \mathbf{q} | \psi \rangle, \\ \langle \mathbf{q} | \hat{p}_r | \psi \rangle &= -i \frac{\partial}{\partial q_r} \psi(\mathbf{q}). \end{aligned} \quad (2.3)$$

A linear operator $\hat{\Gamma}$ on \mathcal{H} (we shall mainly be concerned with bounded operators) is completely determined by its kernel in the Schrödinger representation

$$\Gamma(\mathbf{q}; \mathbf{q}') = \langle \mathbf{q} | \hat{\Gamma} | \mathbf{q}' \rangle. \quad (2.4)$$

The commutation relations (2.1) are invariant under the group of real linear homogeneous symplectic transformations $Sp(2n, \mathbb{R})$. To express these transformations in matrix form, we arrange \hat{q}_r and \hat{p}_r into a column vector \hat{Q} with $2n$ Hermitian operator entries:

$$\hat{Q} = \begin{bmatrix} \hat{q}_1 \\ \vdots \\ \hat{q}_n \\ \hat{p}_1 \\ \vdots \\ \hat{p}_n \end{bmatrix}. \quad (2.5)$$

Then Eq. (2.1) can be compactly written as

$$\begin{aligned} [\hat{Q}_a, \hat{Q}_b] &= i\beta_{ab}, \quad a, b = 1, 2, \dots, 2n \\ \beta &= i\sigma_2 \times \mathbf{1}_{n \times n} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \\ \beta^T &= \beta^{-1} = -\beta. \end{aligned} \quad (2.6)$$

The group $Sp(2n, \mathbb{R})$ consists of $2n$ -dimensional real matrices S obeying

$$S^T \beta S = \beta. \quad (2.7)$$

[It is sometimes useful to note that if $S \in Sp(2n, \mathbb{R})$, then both S^T and S^{-1} belong to $Sp(2n, \mathbb{R})$ as well.] For any $S \in Sp(2n, \mathbb{R})$, if we define operators \hat{Q}'_a by

$$\hat{Q}' = S \hat{Q}, \quad (2.8)$$

it is immediate that \hat{Q}'_a obey the same hermiticity and commutation relations as the \hat{Q}_a . Therefore, there is a unitary operator $U(S)$ determined by S , giving a unitary representation of $Sp(2n, \mathbb{R})$, and carrying \hat{Q}_a to \hat{Q}'_a :

$$\begin{aligned} \hat{Q}'_a &= S_{ab} \hat{Q}_b = U(S)^{-1} \hat{Q}_a U(S), \\ U(S_1) U(S_2) &= U(S_1 S_2). \end{aligned} \quad (2.9)$$

In the Schrödinger representation the effect of $U(S)$ on a wave function $\psi(\mathbf{q})$ is given by a generalized Huyghens integral which for general S involves a nonlocal kernel:

$$\psi'(\mathbf{q}) = \langle \mathbf{q} | U(S) | \psi \rangle = \int d^n q' \langle \mathbf{q} | U(S) | \mathbf{q}' \rangle \psi(\mathbf{q}'). \quad (2.10)$$

The related action on operators $\hat{\Gamma}$ is given by conjugation,

$$\hat{\Gamma}' = U(S)^{-1} \hat{\Gamma} U(S). \quad (2.11)$$

On account of the fundamental significance of the group $Sp(2n, \mathbb{R})$ with respect to the commutation relations (2.1) and (2.6), we can ask if there exists a way of describing operators $\hat{\Gamma}$ such that the action (2.11) becomes as simple as possible.¹⁹ A suggestion as to how this may be achieved is obtained by examining the infinitesimal elements of $Sp(2n, \mathbb{R})$ and generators for $U(S)$. An $S \in Sp(2n, \mathbb{R})$ close to the identity can be expressed as

$$\begin{aligned} S &\simeq 1 + \epsilon J, \quad |\epsilon| \ll 1 \\ (\beta J)^T &= \beta J. \end{aligned} \quad (2.12)$$

The corresponding $U(S)$ must differ from unity by a symmetric quadratic expression in $\hat{\mathbf{Q}}$ since on commutation with $\hat{\mathbf{Q}}$ the result has to be linear in $\hat{\mathbf{Q}}$. A straightforward calculation shows that

$$\begin{aligned} \hat{\mathbf{Q}}'_a &\simeq \hat{\mathbf{Q}}_a + \epsilon J_{ab} \hat{\mathbf{Q}}_b = \hat{\mathbf{Q}}_a + \frac{i}{2} \epsilon [\hat{\mathbf{Q}}^T G \hat{\mathbf{Q}}, \hat{\mathbf{Q}}_a] \\ &\simeq U(S)^{-1} \hat{\mathbf{Q}}_a U(S), \\ U(S) &\simeq 1 - \frac{i}{2} \epsilon \hat{\mathbf{Q}}^T G \hat{\mathbf{Q}}, \\ G &= G^T = -\beta J. \end{aligned} \quad (2.13)$$

The correspondence between commutators among J 's and among symmetric hermitian bilinears $\hat{\mathbf{Q}}^T G \hat{\mathbf{Q}}$ is given by

$$\begin{aligned} \left[-\frac{i}{2} \hat{\mathbf{Q}}^T G \hat{\mathbf{Q}}, -\frac{i}{2} \hat{\mathbf{Q}}^T G' \hat{\mathbf{Q}} \right] &= -\frac{i}{2} \hat{\mathbf{Q}}^T G'' \hat{\mathbf{Q}}, \\ G &= -\beta J, \quad G' = -\beta J', \quad G'' = -\beta J'', \\ J'' &= [J, J']. \end{aligned} \quad (2.14)$$

Now the effect of an infinitesimal transformation $U(S)$ on an operator $\hat{\Gamma}$ can be simplified to the form

$$\begin{aligned} \hat{\Gamma}' &= U(S)^{-1} \hat{\Gamma} U(S) \simeq \hat{\Gamma} + \frac{i}{2} \epsilon [\hat{\mathbf{Q}}^T G \hat{\mathbf{Q}}, \hat{\Gamma}] \\ &= \hat{\Gamma} + \frac{i}{2} \epsilon G_{ab} \{ \hat{\mathbf{Q}}_a, [\hat{\mathbf{Q}}_b, \hat{\Gamma}] \}. \end{aligned} \quad (2.15)$$

This suggests that if we can describe operators $\hat{\Gamma}$ in such a way that the processes of commutation and anticommutation with the basic $\hat{\mathbf{q}}$'s and $\hat{\mathbf{p}}$'s assume a very simple form, then the action (2.11) of $\text{Sp}(2n, \mathbb{R})$ will become equally simple. It is precisely this that is achieved by the Moyal transform description of $\hat{\Gamma}$, as we now show.

Given the operator $\hat{\Gamma}$ on \mathcal{H} , its Moyal transform is a function $W(\mathbf{q}; \mathbf{p})$ defined in terms of the kernel $\Gamma(\mathbf{q}; \mathbf{q}')$ by^{10,11}

$$W(\mathbf{q}; \mathbf{p}) = (2\pi)^{-n} \int d^n q' \Gamma(\mathbf{q} - \frac{1}{2} \mathbf{q}'; \mathbf{q} + \frac{1}{2} \mathbf{q}') \exp(i \mathbf{q}' \cdot \mathbf{p}). \quad (2.16)$$

The inverse is

$$\begin{aligned} \Gamma(\mathbf{q}; \mathbf{q}') &= \int d^n p \ W(\frac{1}{2}(\mathbf{q} + \mathbf{q}'); \mathbf{p}) \exp[-i(\mathbf{q} - \mathbf{q}') \cdot \mathbf{p}]. \\ (2.17) \end{aligned}$$

It is now easy to verify that the transition from $\hat{\Gamma}$ to its anticommutators or commutators with the $\hat{\mathbf{q}}$'s and $\hat{\mathbf{p}}$'s is reflected in very simple changes in $W(\mathbf{q}; \mathbf{p})$. For example,

$$\begin{aligned} \hat{\Gamma} \rightarrow \frac{1}{2} \{ \hat{\mathbf{q}}_r, \hat{\Gamma} \} &\Rightarrow \Gamma(\mathbf{q} - \frac{1}{2} \mathbf{q}'; \mathbf{q} + \frac{1}{2} \mathbf{q}') \\ \rightarrow q_r \Gamma(\mathbf{q} - \frac{1}{2} \mathbf{q}'; \mathbf{q} + \frac{1}{2} \mathbf{q}') & \\ \Rightarrow W(\mathbf{q}; \mathbf{p}) \rightarrow q_r W(\mathbf{q}; \mathbf{p}). \end{aligned} \quad (2.18)$$

In this way, the Moyal transforms of the listed operators are related to the transform of $\hat{\Gamma}$ itself by

$$\begin{aligned} \frac{1}{2} \{ \hat{\mathbf{q}}_r, \hat{\Gamma} \} &\rightarrow q_r W(\mathbf{q}; \mathbf{p}), \\ \frac{1}{2} \{ \hat{\mathbf{p}}_r, \hat{\Gamma} \} &\rightarrow p_r W(\mathbf{q}; \mathbf{p}), \\ [\hat{\mathbf{q}}_r, \hat{\Gamma}] &\rightarrow i \frac{\partial}{\partial p_r} W(\mathbf{q}; \mathbf{p}), \\ [\hat{\mathbf{p}}_r, \hat{\Gamma}] &\rightarrow -i \frac{\partial}{\partial q_r} W(\mathbf{q}; \mathbf{p}). \end{aligned} \quad (2.19)$$

This set of results can be compactly expressed if, to accompany the column vector $\hat{\mathbf{Q}}$ made up of operator entries, we define a c -number column vector \mathbf{Q} as

$$\mathbf{Q} = \begin{bmatrix} q_1 \\ \vdots \\ q_n \\ p_1 \\ \vdots \\ p_n \end{bmatrix}. \quad (2.20)$$

Then the Moyal transform of $\hat{\Gamma}$ can be written as $W(\mathbf{Q})$ and Eqs. (2.19) read

$$\begin{aligned} \frac{1}{2} \{ \hat{\mathbf{Q}}_a, \hat{\Gamma} \} &\rightarrow Q_a W(\mathbf{Q}), \\ [\hat{\mathbf{Q}}_a, \hat{\Gamma}] &\rightarrow i \beta_{ab} \frac{\partial}{\partial Q_b} W(\mathbf{Q}). \end{aligned} \quad (2.21)$$

The change in $W(\mathbf{Q})$ when $\hat{\Gamma}$ suffers the infinitesimal $\text{Sp}(2n, \mathbb{R})$ transformation (2.15) is now easily calculated,

$$\begin{aligned} \hat{\Gamma}' &\simeq \hat{\Gamma} + \frac{i}{2} \epsilon [\hat{\mathbf{Q}}^T G \hat{\mathbf{Q}}, \hat{\Gamma}] \Rightarrow W'(\mathbf{Q}) \simeq W(\mathbf{Q}) + i \epsilon G_{ab} Q_a i \beta_{bc} \frac{\partial}{\partial Q_c} W(\mathbf{Q}) \\ &= W(\mathbf{Q}) + \epsilon Q_a J_{ca} \frac{\partial}{\partial Q_c} W(\mathbf{Q}) \\ &\simeq W(e^{\epsilon J} \mathbf{Q}). \end{aligned} \quad (2.22)$$

Hence, upon integration, we obtain for finite elements on a one-parameter subgroup of $\text{Sp}(2n, \mathbb{R})$, and so for any S ,

$$\begin{aligned} \hat{\Gamma}' &= \exp \left[\frac{i}{2} \hat{\mathbf{Q}}^T G \hat{\mathbf{Q}} \right] \hat{\Gamma} \exp \left[-\frac{i}{2} \hat{\mathbf{Q}}^T G \hat{\mathbf{Q}} \right] \Rightarrow W'(\mathbf{Q}) = W(\exp(J) \mathbf{Q}), \\ \hat{\Gamma}' &= U(S)^{-1} \hat{\Gamma} U(S) \Rightarrow W'(\mathbf{Q}) = W(S \mathbf{Q}). \end{aligned} \quad (2.23)$$

This is the characteristic property of the Moyal transform, with respect to $\mathrm{Sp}(2n, \mathbb{R})$, that we were looking for.

It should be emphasized that the above results are valid irrespective of whether or not $\hat{\Gamma}$ has any specific property such as hermiticity, positivity, or finite trace, and also whether it is the density operator of a quantum state or the cross-spectral density (at a fixed frequency) of some optical field. In case $\hat{\Gamma}$ has one or more of these properties, $W(Q)$ will acquire corresponding additional properties as dictated by the defining integral transform (2.16).

III. GAUSSIAN KERNELS AND THEIR MOYAL TRANSFORMS

We are interested in a special class of operators $\hat{\Gamma}$ on $\mathcal{H} = L^2(\mathbb{R}^n)$ whose Schrödinger kernels have the following Gaussian form:

$$\begin{aligned} \langle \mathbf{q} | \hat{\Gamma} | \mathbf{q}' \rangle &\equiv \Gamma(\mathbf{q}; \mathbf{q}') \\ &= (\det L)^{1/2} \exp \left\{ -\mathbf{q}^T L \mathbf{q} - \mathbf{q}'^T L \mathbf{q}' \right. \\ &\quad - \frac{1}{2} (\mathbf{q} - \mathbf{q}')^T M (\mathbf{q} - \mathbf{q}') \\ &\quad \left. + \frac{i}{2} (\mathbf{q} - \mathbf{q}')^T K (\mathbf{q} + \mathbf{q}') \right\}. \end{aligned} \quad (3.1)$$

Here L , M , and K are real n -dimensional matrices with L and M symmetric, while K is arbitrary. Thus the number of independent real parameters in this family of Gaussian kernels is $n(2n+1)$, which is the same as the dimension of $\mathrm{Sp}(2n, \mathbb{R})$. The reality of L, M, K leads to the hermiticity of $\hat{\Gamma}$:

$$\Gamma(\mathbf{q}; \mathbf{q}')^* = \Gamma(\mathbf{q}'; \mathbf{q}) \iff \hat{\Gamma}^\dagger = \hat{\Gamma}. \quad (3.2)$$

We seek additional conditions on the parameter matrices L, M, K so that $\Gamma(\mathbf{q}; \mathbf{q}')$ could be the kernel of the density operator for some (pure or mixed) quantum state, or the cross-spectral density of some optical field. Given that $\hat{\Gamma}$ is Hermitian, in the quantum-mechanical case the additional conditions are that it should be positive semidefinite, and have *unit* trace; while in the optical context, it is enough to have positive semidefiniteness and *finite* trace corresponding to *finite* total intensity. In analyzing these conditions we will make crucial use of the results of Sec. II, so we need to work with the Moyal transform of $\hat{\Gamma}$. Therefore, we wish to impose three conditions on $\hat{\Gamma}$ which we list thus: (A) the trace of $\hat{\Gamma}$ must be finite, (B) the Moyal transform $W(Q)$ of $\hat{\Gamma}$ must exist, and (C) as an operator on \mathcal{H} , $\hat{\Gamma}$ must be positive semidefinite. It is obvious that each of these properties is separately maintained under the $\mathrm{Sp}(2n, \mathbb{R})$ action (2.11). We shall see that while (A) and (B) are easy to handle, (C) is quite subtle.

Let us first impose condition (A) on $\hat{\Gamma}$. It is that

$$\begin{aligned} \mathrm{Tr} \hat{\Gamma} &\equiv \int d^n q \Gamma(\mathbf{q}; \mathbf{q}) \\ &= (\det L)^{1/2} \int d^n q \exp(-2\mathbf{q}^T L \mathbf{q}) < \infty. \end{aligned} \quad (3.3)$$

We see that L must be positive definite,

$$\text{Property (A)} \iff L > 0. \quad (3.4)$$

This will hereafter be assumed. In anticipation of this, the kernel in Eq. (3.1) has been normalized to have a fixed trace:

$$\mathrm{Tr} \hat{\Gamma} = (\pi/2)^{n/2}. \quad (3.5)$$

Next we turn to condition (B). To calculate $W(Q)$ we need the expression

$$\begin{aligned} \Gamma(\mathbf{q} - \frac{1}{2}\mathbf{q}'; \mathbf{q} + \frac{1}{2}\mathbf{q}') &= (\det L)^{1/2} \\ &\times \exp[-2\mathbf{q}^T L \mathbf{q} - \frac{1}{2}\mathbf{q}'^T (L + M) \mathbf{q}' \\ &\quad - i\mathbf{q}'^T K \mathbf{q}]. \end{aligned} \quad (3.6)$$

It follows that $W(Q)$ will exist if and only if the matrix $L + M$ is positive definite:

$$\text{Property (B)} \iff L + M > 0. \quad (3.7)$$

This too will hereafter be assumed, i.e., we assume without exception in the sequel that we are dealing with kernels (3.1) for which both L and $L + M$ are positive definite matrices. Then $W(Q)$ is

$$\begin{aligned} W(Q) &= (2\pi)^{-n/2} [\det L / \det(L + M)]^{1/2} \\ &\times \exp[-2\mathbf{q}^T L \mathbf{q} \\ &\quad - \frac{1}{2}(\mathbf{p} - K \mathbf{q})^T (L + M)^{-1} (\mathbf{p} - K \mathbf{q})]. \end{aligned} \quad (3.8)$$

The quadratic expression in the exponent is positive definite; it can be disentangled and written in terms of Q , bringing in a real symmetric positive definite $2n$ -dimensional matrix G :

$$2\mathbf{q}^T L \mathbf{q} + \frac{1}{2}(\mathbf{p} - K \mathbf{q})^T (L + M)^{-1} (\mathbf{p} - K \mathbf{q}) = Q^T G Q,$$

$$G = \begin{bmatrix} A & C \\ C^T & B \end{bmatrix}. \quad (3.9)$$

The $n \times n$ blocks A, B, C and the original L, M, K can be expressed in terms of each other:

$$\begin{aligned} A &= 2L + \frac{1}{2}K^T(L + M)^{-1}K, \\ B &= \frac{1}{2}(L + M)^{-1}, \end{aligned} \quad (3.10a)$$

$$\begin{aligned} C &= -\frac{1}{2}K^T(L + M)^{-1}; \\ L &= \frac{1}{2}(A - CB^{-1}C^T), \\ M &= \frac{1}{2}(B^{-1} - A + CB^{-1}C^T), \\ K &= -B^{-1}C^T. \end{aligned} \quad (3.10b)$$

It is also useful to express G in the form

$$G = \begin{bmatrix} 1 & 0 \\ -K & 1 \end{bmatrix}^T \begin{bmatrix} 2L & 0 \\ 0 & \frac{1}{2}(L + M)^{-1} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ -K & 1 \end{bmatrix}. \quad (3.11)$$

From this we see that the positive definiteness of L and $L + M$ is equivalent to the positive definiteness of G :

$$L > 0, L + M > 0 \iff G > 0. \quad (3.12)$$

In this statement, K does not appear at all. Similarly,

from Eq. (3.11) we see that $\det G$ is K independent,

$$\det G = \det L / \det(L + M) > 0. \quad (3.13)$$

The Moyal transform can now be written as

$$W(Q) = (2\pi)^{-n/2} [\det L / \det(L + M)]^{1/2} \exp(-Q^T G Q). \quad (3.14)$$

This analysis of the two properties (A), (B), as applied to operators with kernels (3.1), leads us to define a set of operators $\bar{\mathcal{S}}$ as consisting of precisely all those $\hat{\Gamma}$ for which both (A) and (B) hold:

$$\bar{\mathcal{S}} = \{ \hat{\Gamma} \mid L > 0, L + M > 0 \}. \quad (3.15)$$

It is immediate that the $\text{Sp}(2n, \mathbb{R})$ action (2.11) preserves $\bar{\mathcal{S}}$,

$$\hat{\Gamma} \in \bar{\mathcal{S}} \Rightarrow \hat{\Gamma}' = U(S)^{-1} \hat{\Gamma} U(S) \in \bar{\mathcal{S}}. \quad (3.16)$$

The change in the Moyal transform can be read off from Eq. (2.23)

$$\begin{aligned} W'(Q) &\equiv (2\pi)^{-n/2} [\det L' / \det(L' + M')]^{1/2} \\ &\quad \times \exp(-Q^T G' Q) \\ &= W(SQ), \\ G' &= S^T GS. \end{aligned} \quad (3.17)$$

Towards understanding the implications of imposing property (C) on $\hat{\Gamma}$, we first show that a consequence of this property is that the matrix M must be positive semidefinite. For, if $\hat{\Gamma}$ is positive semidefinite, it has a unique positive semidefinite square root $\hat{\Gamma}^{1/2}$. For any two vectors $\phi, \psi \in \mathcal{H}$, the Schwarz inequality applied to $\hat{\Gamma}^{1/2}\phi, \hat{\Gamma}^{1/2}\psi$ gives

$$|\langle \phi | \hat{\Gamma} | \psi \rangle|^2 \leq \langle \phi | \hat{\Gamma} | \phi \rangle \langle \psi | \hat{\Gamma} | \psi \rangle. \quad (3.18)$$

Going to the limit of ideal basis vectors $|\phi\rangle \rightarrow |\mathbf{q}\rangle$, $|\psi\rangle \rightarrow |\mathbf{q}'\rangle$, this means

$$|\Gamma(\mathbf{q}; \mathbf{q}')|^2 \leq \Gamma(\mathbf{q}; \mathbf{q}) \Gamma(\mathbf{q}'; \mathbf{q}'). \quad (3.19)$$

In the optics context this ensures that the normalized degree of coherence is bounded by unity. Using Eq. (3.1) here, we see that if $\hat{\Gamma}$ is positive semidefinite, then

$$\exp[-(\mathbf{q} - \mathbf{q}')^T M (\mathbf{q} - \mathbf{q}')] \leq 1,$$

i.e.,

$$\text{Property (C)} = > M \geq 0. \quad (3.20)$$

However, this is only a necessary and not a sufficient condition to secure property (C) for $\hat{\Gamma}$: The positive semidefiniteness of M does not exhaust all the consequences of the positive semidefiniteness of $\hat{\Gamma}$, but some more restrictions on L , M , and K remain. Nevertheless, the result (3.20) suffices to show that properties (A) and (C) together imply property (B). If, based on (3.20), we define a set of operators \mathcal{S} by

$$\mathcal{S} = \{ \hat{\Gamma} \mid L > 0, M \geq 0 \}, \quad (3.21)$$

it is true that

$$\mathcal{S} \subset \bar{\mathcal{S}}. \quad (3.22)$$

Unlike $\bar{\mathcal{S}}$, however, it will turn out that \mathcal{S} is not preserved by $\text{Sp}(2n, \mathbb{R})$:

$$\hat{\Gamma} \in \mathcal{S} \not\Rightarrow U(S)^{-1} \hat{\Gamma} U(S) \in \mathcal{S}. \quad (3.23)$$

Indeed, we will later construct a whole family of operators in \mathcal{S} which exhibit this behavior. All this happens because the definition of \mathcal{S} captures properties (A) and (B) but not all of (C).

The set of operators we are really after possess all three properties (A), (B), and (C). Let us call this set \mathcal{S}_+ :

$$\mathcal{S}_+ = \{ \hat{\Gamma} \mid L > 0, L + M > 0, \hat{\Gamma} \geq 0 \}. \quad (3.24)$$

It is clear that \mathcal{S}_+ is preserved by the $\text{Sp}(2n, \mathbb{R})$ action, and is contained in \mathcal{S} :

$$\begin{aligned} \hat{\Gamma} \in \mathcal{S}_+ &\Rightarrow U(S)^{-1} \hat{\Gamma} U(S) \in \mathcal{S}_+, \\ \mathcal{S}_+ &\subset \mathcal{S} \subset \bar{\mathcal{S}}. \end{aligned} \quad (3.25)$$

As already mentioned, the (over)complete set of matrix conditions characterizing elements $\hat{\Gamma}$ in \mathcal{S}_+ is $L > 0$, $L + M > 0$, $M \geq 0$ and some other conditions in which the matrix K also plays a role. We will arrive at these conditions by an indirect analysis involving the structure of orbits in the Lie algebra $\text{Sp}(2n, \mathbb{R})$ under the adjoint action. It is because of the subtlety of these conditions that, as an intermediary step, we have defined above the set of operators \mathcal{S} “halfway” between \mathcal{S}_+ and $\bar{\mathcal{S}}$, even though it is not invariant under the $\text{Sp}(2n, \mathbb{R})$ action.

IV. ORBITS IN $\text{Sp}(2n, \mathbb{R})$ AND POSITIVITY OF $\hat{\Gamma}$

We have shown in Sec. II that conjugation of an operator $\hat{\Gamma}$, specified by $\Gamma(\mathbf{q}; \mathbf{q}')$, by $U(S)$ for any $S \in \text{Sp}(2n, \mathbb{R})$ is reflected in a “point transformation” on the arguments Q of its Moyal transform $W(Q)$. Thus one has the “commutative diagram”

$$\begin{array}{ccc} \hat{\Gamma} = \{ \Gamma(\mathbf{q}; \mathbf{q}') \} & \longrightarrow & W(Q) \\ U(S) \downarrow & & S \downarrow \\ \hat{\Gamma}' = U(S)^{-1} \hat{\Gamma} U(S) & \longrightarrow & W'(Q) = W(SQ). \end{array} \quad (4.1)$$

We now have to express the positive semidefiniteness of $\hat{\Gamma}$, for kernels of the family (3.1), as a set of conditions on the matrices L, M, K or equivalently on the symmetric matrix G in $W(Q)$. In doing this, the above diagram will prove essential.

In Sec. II it was also shown that generator matrices J in the defining representation of $\text{Sp}(2n, \mathbb{R})$, and real symmetric $2n \times 2n$ matrices G , stand in one-to-one correspondence according to Eq. (2.13). Therefore any $\hat{\Gamma}$ in $\bar{\mathcal{S}}$, or \mathcal{S}_+ determines uniquely, via the matrix G appearing in $W(Q)$, some J in the Lie algebra $\text{Sp}(2n, \mathbb{R})$ of $\text{Sp}(2n, \mathbb{R})$. Of course not all J arise in this process since, among other things, G has to be positive definite.

The action of $U(S)$ on \hat{F} results in the change (3.17) in G , which is equivalent to J being transformed according to the adjoint representation of $\mathrm{Sp}(2n, \mathbb{R})$

$$G' = S^T G S \Leftrightarrow J' = S^{-1} J S \quad , \quad (4.2)$$

$$G' = -\beta J' , \quad G = -\beta J \quad .$$

For a given J , as S varies over all of $\mathrm{Sp}(2n, \mathbb{R})$, J' traces out the adjoint orbit of J ; i.e., the orbit $\mathcal{O}(J)$ determined by J is

$$\mathcal{O}(J) = \{J' \mid J' = S^{-1}JS, S \in \mathrm{Sp}(2n, \mathbb{R})\} . \quad (4.3)$$

(With no fear of confusion, this orbit of J may be thought of as the orbit of G as well.) Therefore, the property that $\bar{\mathcal{S}}$ and \mathcal{S}_+ are preserved by $\mathrm{Sp}(2n, \mathbb{R})$, while \mathcal{S} is not, can be conveyed in this way: The set of all $\hat{\Gamma} \in \bar{\mathcal{S}}$ determines some complete set of orbits in $\mathrm{Sp}(2n, \mathbb{R})$; similarly, the set of all $\hat{\Gamma} \in \mathcal{S}_+$ determines some complete set of orbits, in fact, a proper subset of the set determined by $\bar{\mathcal{S}}$; finally, the set of J 's determined by the $\hat{\Gamma}$'s in \mathcal{S} does not make up a complete set of orbits at all.

Given that one has to deal with adjoint orbits in $\mathrm{Sp}(2n, \mathbb{R})$, it is natural to try to find a convenient representative point on each orbit. It is the fact that the matrices S belong to a symplectic, rather than to an orthogonal or unitary group, that makes the situation somewhat difficult to visualize geometrically.²⁰ As a preliminary to tackling the case where G is positive definite [an $\mathrm{Sp}(2n, \mathbb{R})$ invariant property], we make some remarks about the properties of J and G as they run over an orbit.

Let $\mathcal{O}(J_0)$ be the orbit of $J_0 \in \mathrm{Sp}(2n, \mathbb{R})$. As $J = S^{-1}J_0S$ runs over $\mathcal{O}(J_0)$, its spectrum does not change since it undergoes similarity transformations. However, there may be no point on $\mathcal{O}(J_0)$ at which J is diagonal. In fact, if $J \in \mathcal{O}(J_0)$ is diagonal,

$$J = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_{2n}) , \quad (4.4)$$

then the symmetry of βJ requires

$$\lambda_{n+1} = -\lambda_1, \quad \lambda_{n+2} = -\lambda_2, \dots, \lambda_{2n} = -\lambda_n. \quad (4.5)$$

In that case G has the form

$$G = \begin{pmatrix} & & \lambda_1 & & 0 \\ & & | & & | \\ & 0 & | & \lambda_2 & | \\ & & | & & | \\ & & & \ddots & | \\ \lambda_1 & - - - - - & 0 & - - - - - & \lambda_n \\ & & | & & | \\ & \lambda_2 & | & & | \\ & & \ddots & & | \\ 0 & & & \lambda_n & | \end{pmatrix} \quad (4.6)$$

which is indefinite. This means that J is never diagonal on any orbit relevant to the study of $\bar{\mathcal{S}}$ or \mathcal{S}_+ .

In contrast to J , G undergoes the symmetric transformation (4.2), so its spectrum does vary over $\mathcal{O}(J_0)$. However, it is easy to see that the “signature of the spectrum of G ” is invariant. Thus, if G and G' are deter-

mined by two points J and J' on the same orbit $\mathcal{O}(J_0)$, and if G is positive definite, negative definite, indefinite, or has an eigenvalue zero, then G' is likewise positive definite, negative definite, indefinite, or has an eigenvalue zero. In particular, either G is positive definite at *all* points of $\mathcal{O}(J_0)$, or G is not positive definite at *any* point of $\mathcal{O}(J_0)$.

The strategy will now be the following. We first characterize, and find representative points on, all those orbits \mathcal{O} over which G is positive definite: These correspond to all $\hat{\Gamma}$'s in $\bar{\mathcal{S}}$ and will be suitably parametrized. The kernel $\Gamma^{(0)}(\mathbf{q}; \mathbf{q}')$ determined by any of these representative points is quite simple and it is quite easy to impose the condition that $\hat{\Gamma}^{(0)}$ be a positive semidefinite operator on \mathcal{H} . This condition will put restrictions on the parameters labeling the orbits and will therefore select the subset of orbits corresponding to $\hat{\Gamma}$'s in \mathcal{S}_+ . We will then develop a set of conditions directly on a positive definite G to ensure that it "belong to \mathcal{S}_+ ," without having to go to the representative point on its orbit. These are the conditions that have been referred to in Sec. III and in which the matrix K plays an essential role.

The basic result we use is Williamson's theorem:¹⁸ If G is a real symmetric positive definite $2n \times 2n$ matrix, there is a point $G^{(0)}$ on the orbit \mathcal{O} of G such that $G^{(0)}$ is diagonal with, of course, positive diagonal elements:

$$G^{(0)} = \begin{pmatrix} \kappa_1 & & & & & & & \\ & \kappa_2 & & & & & & \\ & & \ddots & & & & & \\ & & & \ddots & & & & \\ & \cdots & \cdots & \cdots & \kappa_n & & & \\ & - & - & - & - & - & - & \\ & & & & & \kappa_1 & & \\ & & & & & & \kappa_2 & \\ & & & & & & & \ddots \\ & & & & & & & \kappa_n \\ \kappa_1 \geq \kappa_2 \geq \cdots \geq \kappa_n & & & & & & & \end{pmatrix} \quad (4.7)$$

Two comments must be made regarding the form of $G^{(0)}$: First, we have arranged $G_{n+r, n+r}^{(0)} = G_{r,r}^{(0)}$ for $r = 1, 2, \dots, n$. This is permissible because within a pair (q_r, p_r) we can scale q_r by a factor γ_r and simultaneously scale p_r by the reciprocal factor γ_r^{-1} , and such scalings carried out independently on each canonical pair are elements of $\text{Sp}(2n, \mathbb{R})$. Second, the interchange of one canonical pair (q_r, p_r) with another (q_s, p_s) is also an $\text{Sp}(2n, \mathbb{R})$ transformation so that we can arrange the κ 's in nonincreasing order. The parameters $\{\kappa_r\}$ are not of course the eigenvalues of a general G on the orbit of $G^{(0)}$. Nevertheless, they do invariantly characterize the entire orbit: While J can never become diagonal on such an orbit, at all points its spectrum consists of $\pm i\kappa_1, \pm i\kappa_2, \dots, \pm i\kappa_n$. Therefore, the orbit determined by $G^{(0)}$ of Eq. (4.7) can be written $\mathcal{O}_{\kappa_1, \kappa_2, \dots, \kappa_n}$ and we can say that, in an obvious sense,

$$\bar{\mathcal{S}} = \left\{ \mathcal{O}_{\kappa_1, \kappa_2, \dots, \kappa_n} \mid \kappa_1 \geq \kappa_2 \geq \dots \geq \kappa_n > 0 \right\}. \quad (4.8)$$

Thus the parameter space of the orbits comprising $\bar{\mathcal{F}}$ is the convex cone $\kappa_1 > \kappa_2 > \dots > \kappa_n > 0$ in the n -dimensional

κ space.

We next ask which subset of the orbits in Eq. (4.8) occur in \mathcal{S}_+ . At the representative point $G^{(0)}$ on $\mathcal{O}_{\kappa_1, \kappa_2, \dots, \kappa_n}$, Eq. (4.7), the submatrices $A^{(0)}$, $B^{(0)}$, and $C^{(0)}$ are

$$A^{(0)} = B^{(0)} = \begin{pmatrix} \kappa_1 & & 0 \\ & \kappa_2 & \\ & & \ddots \\ 0 & & \kappa_n \end{pmatrix}, \quad C^{(0)} = 0. \quad (4.9)$$

Therefore, the matrices $L^{(0)}$, $M^{(0)}$, and $K^{(0)}$ needed for $\Gamma^{(0)}(\mathbf{q}; \mathbf{q}')$ are, from Eq. (3.10),

$$\begin{aligned} L^{(0)} &= \frac{1}{2} \text{diag}(\kappa_1, \kappa_2, \dots, \kappa_n), \\ M^{(0)} &= \frac{1}{2} \text{diag}(\kappa_1^{-1} - \kappa_1, \kappa_2^{-1} - \kappa_2, \dots, \kappa_n^{-1} - \kappa_n), \\ K^{(0)} &= 0. \end{aligned} \quad (4.10)$$

We already know that a necessary condition for $\hat{\Gamma}^{(0)} \geq 0$ is that $M^{(0)}$ must be positive semidefinite. This imposes $\kappa_r \leq 1$ for each r , but since κ_1 is the largest of the κ 's it suffices to say

$$M^{(0)} \geq 0 \iff \kappa_1 \leq 1. \quad (4.11)$$

It now happens that at the point $G^{(0)}$ this condition is also sufficient to ensure $\hat{\Gamma}^{(0)} \geq 0$! For, using the matrices (4.10) we have, apart from a numerical factor

$$\begin{aligned} \Gamma^{(0)}(\mathbf{q}; \mathbf{q}') &\doteq \exp \left[-\frac{1}{2} \sum_{r=1}^n [\kappa_r (q_r^2 + q_r'^2) \right. \\ &\quad \left. + \frac{1}{2} (\kappa_r^{-1} - \kappa_r) (\mathbf{q}_r - \mathbf{q}_r')^2] \right]. \end{aligned} \quad (4.12)$$

If $|\psi\rangle \in \mathcal{H}$, then

$$\begin{aligned} \langle \psi | \hat{\Gamma}^{(0)} | \psi \rangle &= \int \int d^n q \, d^n q' \psi^*(\mathbf{q}) \Gamma^{(0)}(\mathbf{q}; \mathbf{q}') \psi(\mathbf{q}') \\ &= \int \int d^n q \, d^n q' \phi^*(\mathbf{q}) \exp \left[-\frac{1}{4} \sum_{r=1}^n (\kappa_r^{-1} - \kappa_r) (q_r - q_r')^2 \right] \cdot \phi(\mathbf{q}'), \\ \phi(\mathbf{q}) &= \exp \left[-\frac{1}{2} \sum_{r=1}^n \kappa_r q_r^2 \right] \psi(\mathbf{q}). \end{aligned} \quad (4.13)$$

Obviously, $\phi(\mathbf{q})$ is also square integrable since each $\kappa_r > 0$, and the translation-invariant kernel multiplying $\phi(\mathbf{q})^* \phi(\mathbf{q}')$ has a positive semidefinite Fourier transform since each $(\kappa_r^{-1} - \kappa_r) \geq 0$. Consequently, $\langle \psi | \hat{\Gamma}^{(0)} | \psi \rangle$ is non-negative for any ψ , i.e., $\hat{\Gamma}^{(0)}$ is a positive semidefinite operator on \mathcal{H} . Once one has shown that $\hat{\Gamma}^{(0)}$ corresponding to $G^{(0)}$ is in \mathcal{S}_+ , the commutative diagram (4.1) ensures that $\hat{\Gamma}$ determined by any other G on the orbit of $G^{(0)}$ is also in \mathcal{S}_+ . Thus, out of all the orbits appearing in (4.8) and making up \mathcal{S} , only those with $\kappa_1 \leq 1$ are present in \mathcal{S}_+ and correspond to positive semidefinite $\hat{\Gamma}$'s:

$$\mathcal{S}_+ = \{ \mathcal{O}_{\kappa_1, \kappa_2, \dots, \kappa_n} \mid 1 \geq \kappa_1 \geq \kappa_2 \geq \dots \geq \kappa_n > 0 \}. \quad (4.14)$$

We can state this result in the form of a theorem.

The necessary and sufficient conditions for the Hermitian Gaussian kernel (3.1) with parameter matrices L, M, K to represent a density operator in quantum mechanics or a cross-spectral density in optics, or equivalently for the real Gaussian phase-space distribution (3.8) or (3.14) to be a genuine Wigner distribution or Wolf function, are

$$G > 0, \quad \kappa_1 \leq 1, \quad (4.15)$$

where the submatrices A, B, C in G are related to L, M, K by Eq. (3.10) and where κ_1 is the largest diagonal element in the normal form $G^{(0)}$ of G .

It is a consequence of conditions (4.15) that $\det G$ is bounded above by unity. For, any $S \in \text{Sp}(2n, \mathbb{R})$ is unimodular, so that $\det G$ is an $\text{Sp}(2n, \mathbb{R})$ invariant. On the other hand, at the representative point $G^{(0)}$ we have

$$\det G^{(0)} = \prod_{r=1}^n \kappa_r^2. \quad (4.16)$$

It follows that for all fields contained in \mathcal{S}_+ , $\det G \leq 1$. In fact, $\det G = 1$ if and only if $\kappa_r = 1$, $r = 1, 2, \dots, n$. In this case, and only in this case, $\Gamma(\mathbf{q}; \mathbf{q}')$ in Eq. (3.1) becomes (essentially) a projection operator representing a pure quantum state, or in the case of optics a fully coherent field.

It can be appreciated at this stage that, while properties (A) and (B) of Sec. III imposed on $\hat{\Gamma}$ are fully equivalent to the positive definiteness of G [see Eqs. (3.4), (3.7), and (3.12)], a complete and faithful rendering of property (C) is [given properties (A) and (B)]

$$\text{Property (C)} \iff \kappa_1 \leq 1. \quad (4.17)$$

Naturally this is an $\text{Sp}(2n, \mathbb{R})$ invariant statement, since the normal form $G^{(0)}$ of a positive definite G as provided by Williamson's theorem, is unique. However, it is clear that the statement (4.17) is not yet expressed in terms of L, M, K or A, B, C in a directly testable way. It is therefore of interest to ask whether, given $G > 0$, we can express the content of Eq. (4.17) in terms of G directly,

without having to find its normal form. This can indeed be done, in terms of the polynomial $\text{Sp}(2n, \mathbb{R})$ invariants formed out of G , as we now show.

Since $J = \beta G$ undergoes similarity transformations under $\text{Sp}(2n, \mathbb{R})$, we see that the traces of powers of βG are $\text{Sp}(2n, \mathbb{R})$ invariants. On an orbit with $G > 0$, Williamson's Theorem allows us to calculate these invariants by going to the normal form $G^{(0)}$:

$$\text{Tr}(\beta G)^m = \begin{cases} 0, & m \text{ odd} \\ 2 \times (-1)^{m/2} \sum_{r=1}^n \kappa_r^m, & m \text{ even} \end{cases} \quad (4.18)$$

That is, the nonzero invariant traces are equal to the sums of various powers of κ_r^2 . We define

$$S_l = \frac{(-1)^l}{2} \text{Tr}(\beta G)^{2l} = \sum_{r=1}^n \kappa_r^{2l}, \quad l = 1, 2, \dots, n, \quad (4.19)$$

and in terms of S_l ,

$$\begin{aligned} C_1 &= -S_1, \\ C_2 &= -\frac{1}{2}(S_2 + C_1 S_1), \\ C_3 &= -\frac{1}{3}(S_3 + C_1 S_2 + C_2 S_1), \\ C_n &= -\frac{1}{n}(S_n + C_1 S_{n-1} + C_2 S_{n-2} + \dots + C_{n-1} S_1). \end{aligned} \quad (4.20)$$

We now form the n th degree polynomial equation with C 's as coefficients:

$$P(y) \equiv y^n + C_1 y^{n-1} + C_2 y^{n-2} + \dots + C_{n-1} y + C_n = 0. \quad (4.21)$$

By Bôcher's theorem,²¹ the roots of this equation are $\kappa_r^2, r = 1, 2, \dots, n$. Since G is positive definite, we know in advance again from Williamson's theorem that when the quantities S_l and then C_l are formed from G and the equation (4.21) is set up, all the roots will be positive definite. Thus to impose the condition $\kappa_1 \leq 1$ which is the same as $\kappa_1^2 \leq 1$, we have to state the conditions under which all the roots of Eq. (4.21) are less than or equal to unity. Suppose

$$P(1), \left[\frac{dP(y)}{dy} \right]_{y=1}, \dots, \left[\frac{d^{n-1}P(y)}{dy^{n-1}} \right]_{y=1} \geq 0. \quad (4.22)$$

Then $P(y) > 0$ for all $y > 1$ [as is easily seen by making a Taylor expansion of $P(y)$ about $y = 1$], implying that there are no roots of (4.21) beyond $y = 1$. Conversely, if (4.21) has no roots beyond $y = 1$, the inequalities (4.22) follow from writing $P(y)$ in the factored form

$$P(y) \equiv (y - \kappa_1^2)(y - \kappa_2^2) \cdots (y - \kappa_n^2). \quad (4.23)$$

Thus we have proved that the inequalities (4.22), n in number, are the necessary and sufficient conditions to ensure that $\kappa_1 \leq 1$, given the positive definiteness of G and hence the validity of Williamson's theorem. Written

explicitly in terms of the C 's these inequalities are

$$\begin{aligned} 1 + C_1 + C_2 + \dots + C_n &\geq 0, \\ n + (n-1)C_1 + (n-2)C_2 + \dots + 2C_{n-2} + C_{n-1} &\geq 0, \\ n(n-1) + (n-1)(n-2)C_1 + \dots + 6C_{n-3} + 2C_{n-2} &\geq 0, \\ n! + (n-1)!C_1 &\geq 0. \end{aligned} \quad (4.24)$$

Thus we have an explicitly $\text{Sp}(2n, \mathbb{R})$ invariant algorithm to impose the crucial condition $\kappa_1 \leq 1$ on a given G without having to put it into its normal form: Starting with a positive definite G , we compute the traces of the first n even powers of βG . We use these traces to form S_l and from them the C_l via Eqs. (4.19) and (4.20). We then form the n linear combinations of the C_l appearing in (4.24). If all of these are non-negative, then $\kappa_1 \leq 1$; otherwise, $\kappa_1 > 1$. At least the last of these inequalities is quite transparent: It merely says that $-C_1$, which is the sum $\kappa_1^2 + \kappa_2^2 + \dots + \kappa_n^2$, must not exceed n .

The above results derived for n canonical pairs of variables are relevant as they stand in quantum mechanics. However, in the context of paraxial propagation problems in optics, the cases of direct relevance are $n = 1$ and $n = 2$, corresponding, respectively, to isotropic and anisotropic Gaussian Schell-model beams. We therefore illustrate the general results by specializing to the cases $n = 1, 2$.

Case of $n = 1$. The relevant symplectic group is $\text{Sp}(2, \mathbb{R})$ which is isomorphic to $\text{SL}(2, \mathbb{R})$ and is a twofold covering group of $\text{SO}(2, 1)$.¹² The normal form of G is, given its positive definiteness,

$$G^{(0)} = \begin{bmatrix} \kappa & 0 \\ 0 & \kappa \end{bmatrix}, \quad \kappa > 0. \quad (4.25)$$

There is only one algebraic invariant, namely,

$$S_1 = -C_1 = -\frac{1}{2} \text{Tr}(\beta G)^2 = \kappa^2. \quad (4.26)$$

Operators $\hat{\Gamma} \in \bar{\mathcal{S}}$ determine a one-parameter family of orbits $\mathcal{O}_\kappa, \kappa > 0$, in the three-dimensional Lie algebra $\text{Sp}(2, \mathbb{R})$; each such $\hat{\Gamma}$ has a Gaussian kernel (3.1) with $n = 1$, a finite trace, and a finite Moyal transform. The matrices J making up the orbit \mathcal{O}_κ are evidently

$$\mathcal{O}_\kappa = \{i\kappa S^{-1} \sigma_2 S \mid S \in \text{Sp}(2, \mathbb{R})\}. \quad (4.27)$$

To determine which subset of the orbits \mathcal{O}_κ for $\kappa > 0$ correspond to \mathcal{S}_+ , we have to impose the inequality in the first line of Eqs. (4.24). Thus we see that only \mathcal{O}_κ for $\kappa \leq 1$ arises in correspondence with the positive semidefinite $\hat{\Gamma}$'s comprising \mathcal{S}_+ . In this simple case with $n = 1$, since $\det G = \kappa^2$, the condition $\det G \leq 1$ already ensures $\kappa \leq 1$ and so the positive semidefiniteness of $\hat{\Gamma}$.

Case of $n = 2$. In this case the symplectic group is $\text{Sp}(4, \mathbb{R})$ which is a twofold covering of $\text{SO}(3, 2)$. Based on this fact, we have elsewhere made a complete listing of all orbits that arise in the ten-dimensional Lie algebra $\text{Sp}(4, \mathbb{R})$ as corresponding to real symmetric positive definite 4×4 matrices G .¹³ Those same results are immediately recovered from the present analysis. Two pa-

rameters κ_1, κ_2 are needed to label the relevant orbits, and the normal form of a positive definite G is

$$G^{(0)} = \begin{pmatrix} \kappa_1 & & 0 \\ & \kappa_2 & \\ & & \kappa_1 \\ 0 & & \kappa_2 \end{pmatrix}, \quad \kappa_1 \geq \kappa_2 > 0. \quad (4.28)$$

This $G^{(0)}$ determines a $J^{(0)} \in \text{Sp}(4, \mathbb{R})$ whose orbit is $\mathcal{O}_{\kappa_1, \kappa_2}$. Our analysis based on $\text{SO}(3,2)$ has shown that the case $\kappa_1 = \kappa_2$ is to be distinguished from the case $\kappa_1 > \kappa_2$ because the natures of the J 's in the two cases are rather different. Thus we prefer to exhibit $\bar{\mathcal{S}}$ as

$$\begin{aligned} \bar{\mathcal{S}} &= \{\mathcal{O}_{\kappa_1, \kappa_2} \mid \kappa_1 \geq \kappa_2 > 0\} \\ &= \{\mathcal{O}_{\kappa, \kappa} \mid \kappa > 0\} \cup \{\mathcal{O}_{\kappa_1, \kappa_2} \mid \kappa_1 > \kappa_2 > 0\}, \end{aligned} \quad (4.29)$$

and call these two families of orbits as types I and II, respectively. In order to find what part of \mathcal{S} makes up \mathcal{S}_+ , we must impose two inequalities corresponding to the first two lines of (4.24). In types I and II, respectively, we have

$$\begin{aligned} \mathcal{O}_{\kappa, \kappa}: C_1 &= -2\kappa^2, \quad C_2 = \kappa^4. \\ \mathcal{O}_{\kappa_1, \kappa_2}: C_1 &= -\kappa_1^2 - \kappa_2^2, \quad C_2 = \kappa_1^2 \kappa_2^2, \end{aligned} \quad (4.30)$$

while the relevant inequalities are

$$-C_1 \leq 2, \quad -C_1 - C_2 \leq 1. \quad (4.31)$$

Therefore, the orbits corresponding to positive semidefinite $\hat{\Gamma}$'s in \mathcal{S}_+ are

$$\mathcal{S}_+ = \{\mathcal{O}_{\kappa, \kappa} \mid 1 \geq \kappa > 0\} \cup \{\mathcal{O}_{\kappa_1, \kappa_2} \mid 1 \geq \kappa_1 > \kappa_2 > 0\}. \quad (4.32)$$

The increase in complexity as compared to the case $n = 1$ is seen in the following fact: While $\det G = \kappa_1^2 \kappa_2^2$ is bounded above by unity as long as one observes the limit $\kappa_1 \leq 1$, the condition $\det G \leq 1$ is no longer sufficient to ensure that $\hat{\Gamma}$ be positive semidefinite. Therefore, the conditions for G to "belong to \mathcal{S}_+ " have to be written as the pair of inequalities.

$$\begin{aligned} -\text{Tr}(\beta G)^2 &\leq 4, \\ 2 \text{Tr}(\beta G)^4 - [\text{Tr}(\beta G)^2]^2 - 4 \text{Tr}(\beta G)^2 &\leq 8, \end{aligned} \quad (4.33)$$

and these imply, but are not implied by, $\det G \leq 1$. Every $\hat{\Gamma}$ for a system with $n = 2$, which is Hermitian, has finite trace, a finite Moyal transform, and is positive semidefinite is given by a real positive definite 4×4 matrix G obeying the $\text{Sp}(4, \mathbb{R})$ -invariant inequalities (4.33).

V. ROLE OF THE PHASE MATRIX K

It has been emphasized in earlier sections that while the matrix K determining the phase of the Gaussian kernel (3.1) plays no role in implementing properties (A) on (B) of Sec. III on $\hat{\Gamma}$, it does play an essential role where property (C) is concerned. We now study this aspect in more detail.

It is first important to recognize that the symmetric part of K is again irrelevant as far as property (C), i.e., the positive semidefiniteness of $\hat{\Gamma}$, is concerned. At the level of the kernel (3.1) we see that when K is split into its symmetric and antisymmetric parts, K_s and K_a , the former contributes a phase factor separable in \mathbf{q} and \mathbf{q}' :

$$K = K_s + K_a,$$

$$\exp \left[\frac{i}{2} (\mathbf{q} - \mathbf{q}')^T K (\mathbf{q} + \mathbf{q}') \right] = \exp \left[\frac{i}{2} \mathbf{q}^T K_s \mathbf{q} \right] \exp(i \mathbf{q}^T K_a \mathbf{q}') \exp \left[-\frac{i}{2} \mathbf{q}'^T K_s \mathbf{q}' \right]. \quad (5.1)$$

Therefore, the K_s -dependent part can be removed by a unitary transformation on Γ , resulting in a $\hat{\Gamma}'$ for which K is purely antisymmetric. In fact, this unitary transformation is $U(S)$ for a certain $S \in \text{Sp}(2n, \mathbb{R})$ determined by K_s . Following the notation of Eq. (3.16) one has

$$\begin{aligned} \hat{\Gamma}' &= U(S) \hat{\Gamma}' U(S)^{-1}, \quad U(S) = \exp \left[\frac{i}{2} \hat{\mathbf{q}}^T K_s \hat{\mathbf{q}} \right], \\ S &= \begin{pmatrix} \mathbf{1} & 0 \\ K_s & \mathbf{1} \end{pmatrix}, \end{aligned} \quad (5.2)$$

$$\Gamma'(\mathbf{q}; \mathbf{q}') = (\det L)^{1/2} \exp[-\mathbf{q}^T L \mathbf{q} - \mathbf{q}'^T L \mathbf{q}' - \frac{1}{2}(\mathbf{q} - \mathbf{q}')^T M(\mathbf{q} - \mathbf{q}') + i \mathbf{q}^T K_a \mathbf{q}'].$$

This identification of $S \in \text{Sp}(2n, \mathbb{R})$ is seen to be correct by working at the level of the matrix G and expanding Eq. (3.11) to the form

$$G = \begin{pmatrix} \mathbf{1} & 0 \\ -K_s & \mathbf{1} \end{pmatrix}^T \begin{pmatrix} \mathbf{1} & 0 \\ -K_a & \mathbf{1} \end{pmatrix}^T \begin{pmatrix} 2L & 0 \\ 0 & \frac{1}{2}(L + M)^{-1} \end{pmatrix} \begin{pmatrix} \mathbf{1} & 0 \\ -K_a & \mathbf{1} \end{pmatrix} \begin{pmatrix} \mathbf{1} & 0 \\ -K_s & \mathbf{1} \end{pmatrix}. \quad (5.3)$$

The factors involving K_s obey the condition (2.7) and so belong to the defining representation of $\text{Sp}(2n, \mathbb{R})$, while the K_a -dependent factors do not. Comparing Eq. (5.3) with Eqs. (3.16) and (3.17) leads to the S given in Eq. (5.2). We see now that $\hat{\Gamma}$ is positive semidefinite if $\hat{\Gamma}$ is, and conversely. Therefore, the set of n inequalities (4.24) which are equivalent to the condition $\kappa_1 \leq 1$, and which in turn express the condition that $\hat{\Gamma}$ be positive semidefinite, can involve only K_a and not K_s . In passing we note that $U(S)$ in Eq. (5.2) corresponds to a lens action in the context of optics ($n=1, 2$), and to an impulsive harmonic potential in the context of quantum evolution.

Of the full set of n inequalities (4.24) that must be imposed on G to secure property (C) for $\hat{\Gamma}$, the last one,

$$n + C_1 \geq 0, \quad (5.4)$$

is relevant for all $n \geq 1$; the previous one,

$$\frac{1}{2}n(n-1) + (n-1)C_1 + C_2 \geq 0, \quad (5.5)$$

is relevant for all $n \geq 2$, and so on. Each of the conditions (4.24) does involve K_a , but we shall here bring out the weakest restriction on K_a contained in (5.4), the condition relevant for all n values. From Eqs. (4.19) and (4.20) defining C_1 and Eqs. (3.9) and (3.10), we have

$$\begin{aligned} -C_1 &= -\frac{1}{2} \text{Tr}(\beta G)^2 \\ &= \text{Tr}(AB - C^2) \\ &= \text{Tr}L(L + M)^{-1} \\ &\quad + \frac{1}{4} \text{Tr}K^T(L + M)^{-1}(K - K^T)(L + M)^{-1}. \end{aligned} \quad (5.6)$$

Since both L and $L + M$ are assumed to be positive definite, there is a unique symmetric real positive definite matrix $(L + M)^{-1/2}$, and the second trace term can be seen to actually involve only $K - K^T$; we can then put $-C_1$ into the compact form

$$\begin{aligned} -C_1 &= \text{Tr}L(L + M)^{-1} + \frac{1}{2} \text{Tr}N^TN, \\ N &= (L + M)^{-1/2}K_a(L + M)^{-1/2}. \end{aligned} \quad (5.7)$$

Therefore, the weakest condition on K_a is this:

$$\text{Tr}L(L + M)^{-1} + \frac{1}{2} \text{Tr}N^TN \leq n. \quad (5.8)$$

For $n=1$, this is empty since K_a vanishes but for $n \geq 2$ we have a definite restriction on K_a which prevents it from being "too large." As an example, if $M=0$, any nonzero K_a immediately violates the condition (5.8). Thus for any K_a however small but nonzero, the Hermitian operator $\hat{\Gamma}$ with the kernel

$$\Gamma(\mathbf{q}; \mathbf{q}') = \exp(-\mathbf{q}^T L \mathbf{q} - \mathbf{q}'^T L \mathbf{q}' + i \mathbf{q}^T K_a \mathbf{q}') \quad (5.9)$$

is certainly not positive semidefinite. Returning to the general case, the remaining inequalities in (4.34) can be expected to put further restrictions on K_a beyond (5.8).

We take the opportunity now to point out and rectify an incompleteness in the analysis of anisotropic Gaussian Schell-model fields presented in Ref. (15). In that work one is concerned with $n=2$, and the conditions

imposed on the matrix G were the following:

$$\begin{aligned} G &> 0, \\ \det G &< 1, \\ 2M &= B^{-1} - A + CB^{-1}C^T \geq 0. \end{aligned} \quad (5.10)$$

It was then stated that any such G defines an acceptable optical field of the AGSM type. The incompleteness consists in not recognizing that $M \geq 0$ is only a necessary condition for $\hat{\Gamma}$ to be positive semidefinite and not a sufficient one. The subtle role of K , the matrix determining the phase of $\Gamma(\mathbf{q}; \mathbf{q}')$, was not realized in Ref. (15). Apart from this, however, the fact that allowed AGSM fields can be classified into two types, as shown in Eq. (4.32), with $0 < \kappa \leq 1$ in type I and $0 < \kappa_2 < \kappa_1 \leq 1$ in type II, is exactly as was found in Ref. 15.

Finally, we turn to the promised demonstration of the fact that the set \mathcal{S} of operators $\hat{\Gamma}$ defined by Eq. (3.21) is not $\text{Sp}(2n, \mathbb{R})$ invariant. For this we consider a positive definite matrix G with $L > 0$, $M=0$, and $K=K_a \neq 0$. The corresponding operator $\hat{\Gamma}$ definitely belongs to \mathcal{S} but is not positive semidefinite since the condition (5.8) is violated. Now by Williamson's theorem we can transform G to its normal form $G^{(0)}$ and it will then happen that $\kappa_1 > 1$. This implies by Eq. (4.10) that the matrix $M^{(0)}$ corresponding to $G^{(0)}$ has at least one negative eigenvalue, that is, $M^{(0)}$ is not positive semidefinite. Therefore, $\hat{\Gamma}^{(0)}$ determined by $G^{(0)}$ does not belong to \mathcal{S} . At the same time $\hat{\Gamma}$ and $\hat{\Gamma}^{(0)}$ are unitarily related by $U(S)$ for the S needed to take G to its normal form $G^{(0)}$. This establishes that \mathcal{S} is not $\text{Sp}(2n, \mathbb{R})$ invariant.

VI. CONCLUDING REMARKS

We have presented in this paper a systematic analysis of configuration-space Gaussian density kernels and their associated Moyal transforms which are also Gaussian. The former are parametrized by the matrices L, M, K and the latter by the matrix G , and we have allowed the "number of degrees of freedom" $2n$ to be quite general. Given a Gaussian phase-space distribution characterized by the matrix G , the necessary and sufficient conditions for it to be a Wigner distribution have been shown to be that (i) the matrix G must be positive definite, and (ii) the traces of $(\beta G)^{2l}$ for $l=1, 2, \dots, n$ must obey the n inequalities (4.24). These conditions are manifestly $\text{Sp}(2n, \mathbb{R})$ invariant. In this connection we may point out that it is deceptive to view the condition $\kappa_1 \leq 1$, appearing in Eqs. (4.15) and (4.17) as an expression of property (C), as constituting "just one condition," since it has to apply to the largest of the κ 's that appear in the normal form $G^{(0)}$ of G . A more complete statement involving all the κ 's and not relying on the verbal instruction to pick out the largest of them would be

$$\text{Property (C)} \iff \kappa_r \leq 1, \quad r = 1, 2, \dots, n. \quad (6.1)$$

In this form we do have n inequalities, and their expression directly in terms of the $\text{Sp}(2n, \mathbb{R})$ invariants of G is in (4.24).

The analysis and results have both been presented in such a way as to be readily applicable to both quantum

mechanics and optics. It is useful to have a physical interpretation of the $\text{Sp}(2n, \mathbb{R})$ invariant κ 's appearing in the normal form (4.7). In the optical GSM case, $n=1$, there is only one κ which coincides with $(\det G)^{1/2}$, and it has been shown¹² that it is the well-known degree of global coherence defined as the ratio of the transverse coherence length to the intensity width.²² In the AGSM case, $n=2$, there are two κ 's (which coincide for the type-I fields), and a similar physical interpretation has been established. In the context of quantum mechanics we have already noted in the Introduction that the Gaussian Wigner distributions correspond to thermal states of harmonic oscillator systems, and their transforms under $\text{Sp}(2n, \mathbb{R})$. For a one-dimensional oscillator ($n=1$) of frequency ω the Wigner distribution of the thermal state at temperature T is given by the familiar Gaussian expression²³

$$W(\mathbf{q}; \mathbf{p}) \doteq \exp \left[-\tanh(\omega/2k_B T) \left[m\omega q^2 + \frac{p^2}{m\omega} \right] \right]. \quad (6.2)$$

This means that G in this case is the 2×2 matrix

$$G = \tanh(\omega/2k_B T) \begin{bmatrix} m\omega & 0 \\ 0 & 1/m\omega \end{bmatrix}, \quad (6.3)$$

so that

$$\kappa = (\det G)^{1/2} = \tanh(\omega/2k_B T). \quad (6.4)$$

Thus the invariant κ is essentially the ratio of the natural frequency of the oscillator to the temperature, and this is a symplectic invariant. For $n > 1$ we note from Eq. (4.12) that in its normal form the configuration-space kernel is separable in the n degrees of freedom, so the various κ 's give the n -invariant ω/T ratios.

As a final remark we wish to point out that the analysis of this paper can be profitably used to study the problem of squeezed states²⁴ in a multimode system. This is because the G matrix is the inverse of the variance matrix and the squeezing operator is an $\text{Sp}(2n, \mathbb{R})$ transformation. Thus the transformation law for G under $\text{Sp}(2n, \mathbb{R})$ as given in this paper contains as a special case the transformation law of the variances under squeezing.²⁵ We plan to return to this problem elsewhere.

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