Journal of Mathematical Chemistry (2023) 61:277–287
https://doi.org/10.1007/s10910-022-01355-6

BRIEF COMMUNICATION

Semiclassical and thermal phase space entropies measuring complexity

Imre Varga[1]

Received: 7 March 2022 / Accepted: 13 April 2022 / Published online: 19 May 2022

Abstract

Measures of delocalization in phase space are analyzed using Rényi entropies, especially two of which play an important role in characterizing extension and shape of distributions: the linear entropy related to the participation number and the Shannon-entropy. The difference of these two, termed as structural entropy, has been successfully applied in a large variety of physical situations and for various mathematical problems. A very similar quantity has coincidentally been used as a measure of complexity by some other authors. Hereby we show that various semiclassical phase space representations of quantum states can be well described by the structural entropy providing a transparent picture in relation to the thermodynamic description. Thermodynamic and quantum fluctuations are analytically treated for the special case of harmonic oscillators invoking the Einstein model of heat capacity. It is demonstrated that the thermal uncertainty relations are linked to the delocalization over the phase space. For respective limits of zero temperature implying quantum behavior or infinite temperature implying classical behavior we also show which quantities remain useful. As a byproduct the thermal extension of the phase space distribution can be calculated that is directly related to a decoherence parameter introduced by Zurek in a different context.

Keywords Rényi entropy · Complexity · Structural entropy · Phase space · Harmonic oscillator

Dedicated to the memory of János Pipek

✉ Imre Varga
varga.imre@ttk.bme.hu

[1] Department of Theoretical Physics, Institute of Physics, Budapest University of Technology and Economics, Műegyetem rkp. 3., Budapest 1111, Hungary

1 Introduction

Investigation of quantum systems in phase space provides further insight as compared to the real space or momentum space marginals. A quantum sate in principle is completely given in any of the latter two representations with the Fourier transformation connecting one to the another. However, especially in the case of systems with a Hamiltonian that is a combination of terms with real space and momentum space eigenbasis the interplay of these terms reveal finer details in case of investigating in phase space as has been presented in an earlier paper of ours [1], where we have applied an analysis first introduced and widely used by Pipek and coworkers [2–14]. The analysis developed for any type of distributions is based on their information content and their spread over the available basis. Not only the effective size of these distributions but also its shape, especially the deviations from uniformity has been put together. There has been a continuous interest in the application of these methods developed earlier. The most recent applications include Vogel spirals [15], and Colonscopy Image Processing with fuzzy inference optimization in the selection of the rulebase parameters [16, 17], just to select a few.

Coincidentally there has been a development of the so-called complexity analysis of distributions starting from the early work of López-Ruiz, Mancini and Colbet (LMC) [18, 19]. That idea was extended by a very wide range of papers and later on López-Ruiz [20] noticed the direct and simple relation between Pipek's parameters and the one termed as LMC complexity. Apparently the structural entropy introduced by Pipek and coworkers is nothing else but the log of LMC, hence both are equivalent and in most cases provide very similar or in some cases complementer answers to the questions of complexity and shape analysis. The definition of structural entropy has a somewhat more solid mathematical basis using Rényi entropies [21].

In the subsequent part we first outline the model and phase space quantities under consideration, then in the next part provide analogous quantities based on a thermal formulation. In a further section we discuss the thermal uncertainty in phase space and the final section is left for conclusions.

2 The model and phase space quantities

The example we work out in detail is the textbook problem of a linear harmonic oscillator (HO). Its simplicity allows for a transparent application and analysis of the questions formulated above together with an analytical treatment providing simple results in closed form. Moreover, this analysis is directly connected to the study of the Einstein solid and its thermodynamic properties, thus allowing for a direct connection between thermodynamic and quantum mechanical and semiclassical phase space formulation. This part follows similar analysis but goes beyond the one presented in the papers by Penin [22–25]. For more details, please, refer to those papers and the references cited there.

On the other hand the eigenstates of the HO play an important role in the definition of coherent states which are essential in the phase space mapping of quantum systems, hence in the understanding of the correspondence between the classical and quantum realms including the phenomenon of decoherence.

Let us start already with the phase space representation of a harmonic oscillator at finite temperature, $T > 0$,

$$\mu_\beta(x, p) = \langle z|\rho|z\rangle, \tag{1}$$

through the matrix element of the density operator, ρ, using the complex coordinates z related to (x, p) of phase space as

$$z = \frac{1}{2}\left(\frac{x}{\sigma_x} + i\frac{p}{\sigma_p}\right), \tag{2}$$

where σ_x and σ_p are either certain broadenings connected through the uncertainty, $\sigma_x\sigma_p = \hbar$. The ρ is defined as

$$\rho = \frac{1}{Z}e^{-\beta H} \tag{3}$$

with Z being the partition sum in the form of

$$Z = \mathrm{Tr}\left\{e^{-\beta H}\right\}. \tag{4}$$

In these expressions temperature appears through $\beta = (k_B T)^{-1}$, which is the usual inverse temperature where k_B is Boltzmann's constant.

The Hamiltonian, H, in our case is given as

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2. \tag{5}$$

The solution of the eigenvalue equation $H|n\rangle = E_n|n\rangle$ yields the eigenenergies

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right), \tag{6}$$

The matrix elements of the density operator in Eq. (1) can be calculated using the eigenstates $|n\rangle$ with the result

$$\mu_\beta(z) = \frac{1}{Z}\sum_n e^{-\beta E_n} |\langle z|n\rangle|^2, \tag{7}$$

which is nothing else, but the Husimi function [26–28] representation of the density operator ρ over phase space. Hereby we can specify the parameters in Eq. (2) as $\sigma_x = \sqrt{2\hbar/m\omega}$. Since

$$|\langle z|n\rangle|^2 = \frac{|z|^{2n}}{n!}e^{-|z|^2}, \tag{8}$$

therefore the closed form for Eq. (1) reads as [29, 30]

$$\mu_\beta(z) = (1 - e^{-\beta\hbar\omega})e^{-(1-e^{-\beta\hbar\omega})|z|^2}. \tag{9}$$

This is a density over the phase space which is normalized as

$$\int\int \frac{dxdp}{2\pi\hbar}\mu_\beta(x,p) = 1. \tag{10}$$

The great advantage of the analysis of HO states is that the partition sum can readily be calculated and expressed as a function of $\beta\hbar\omega$ in a closed form as

$$Z(\beta) = \left[2\sinh\left(\frac{\beta\hbar\omega}{2}\right)\right]^{-1}. \tag{11}$$

This expression allows for further thermodynamic definitions of entropy, S_T, the mean energy, U, and the specific heat, C_V, respectively, which we will look at later.

This is the point where we should mention the Einstein solid, the first model of heat capacity. In that case the partition sum of the system of N lattice sites in a $d = 3$ dimensional solid is nothing else but the product of $3N$ HOs given in Eq. (11),

$$Z_N(\beta) = \left[2\sinh\left(\frac{\beta\hbar\omega}{2}\right)\right]^{-3N}. \tag{12}$$

therefore all types of entropies introduced from now on are nothing else but the entropies obtained for the solid divided by $3Nk_B$.

In order to characterize the properties of this phase space distribution we may introduce various measures. First the measure of its extension can be defined using the participation number,

$$D_H^{-1} = \int\int \frac{dxdp}{2\pi\hbar}\mu_\beta^2(x,p), \tag{13}$$

We introduced the index H which stands for Husimi, emphasizing that the above representation of the density matrix Eq. (9) is nothing else but the Husimi function, i.e., the coherent state representation of the density operator in Eq. (1). For a similar purpose Wehrl introduced the entropy [31] in analogy with the Shannon–entropy

$$I_W = -\int\int \frac{dxdp}{2\pi\hbar}\mu_\beta(x,p)\ln\mu_\beta(x,p), \tag{14}$$

with a lower bound noticed by Lieb [32]. Using Eq. (9) in these definitions we get

$$D_H^{-1} = \frac{1}{2}\left(1 - e^{-\beta\hbar\omega}\right), \tag{15}$$

which gives a direct and thermal measure of localization of the Husimi function in phase space. The same way we obtain the Wehrl entropy in a closed form

$$I_W = 1 - \ln\left(1 - e^{-\beta\hbar\omega}\right). \tag{16}$$

We have to emphasize that Wehrl's entropy and the extension, D_H, are both special cases of Rényi's entropies of the Husimi function [1] which can be defined as

$$R_q^{(H)} = \frac{1}{1-q} \ln \int \int \frac{dxdp}{2\pi\hbar} \mu_\beta^q(x, p). \tag{17}$$

Note that in all of the above entropy like definitions and generalizations Boltzmann's constant, k_B is supposed to multiply these quantities. Using the phase space representation of the HO, Eq. (9), we obtain a simple closed from of the integral in Eq. (17)

$$\int \int \frac{dxdp}{2\pi\hbar} \mu_\beta^q(x, p) = `\frac{1}{q} \left(1 - e^{-\beta\hbar\omega}\right)^{q-1}. \tag{18}$$

Therefore the Rényi–entropies can be evaluated as

$$R_q^{(H)} = -\ln\left(1 - e^{-\beta\hbar\omega}\right) - \frac{\ln q}{1-q}. \tag{19}$$

In the limit of $q \to 1$ this definition yields the Wehrl–entropy, I_W, (see Eq. (16)) and for $q = 2$ we get $R_2^{(H)} = \ln D_H$. On the other hand, exponentiating these values of R_q we get the extensions at different orders, i.e., the qth order moments of the distribution. We also have to note that D_H^{-1} is also termed as purity which is related to the so called linear entropy.

Apart from being generalizations of the Wehrl–entropy, the Rényi–entopries have some further valuable properties which were exploited in a number of previous works. Not only the extension but also the distribution under investigation may be characterized using a special combination of these entropies. In Ref. [1] the structural entropy, S_{str}, has been introduced for phase space distributions. This quantity is nonnegative and can be calculated as a difference of the Shannon–entropy, $R_1^{(H)} = I_W$, and the extension entropy, $R_2^{(H)} = \ln D_H$ as

$$S_{str}^{(H)} = I_W - \ln D_H. \tag{20}$$

This definition can obviously be extended and applied in any other case. In the present investigation using Eqs. (15) and (16), we get

$$S_{str}^{(H)} = 1 - \ln 2 \ , \tag{21}$$

which shows that the phase space distirbution here for the case of the HO, has an overall Gaussian shape (see Eq. 9) over a two dimensional phase space. The fact that $S_{str}^{(H)}$ is independent from the value of $\beta\hbar\omega$ can be readily seen from the expression Eq. (19).

Notice that for the case of a HO one could investigate another widely applied phase space distribution introduced by Wigner[33], which in general does not yield a nonnegative phase space distribution like the Husimi function but at least its x and p

marginals are nothing else but the correct real space and momentum space distributions of the density operator or the eigenstates of the system. In the present case of HO, however, the Wigner function yields a slightly different Gaussian form that is still a nonnegative distribution.

3 Thermodynamic quantities

Now we turn to thermodynamic quantities using the expression of the partition sum (11) and define first the entropy, S_T as

$$S_T = \ln Z - \frac{d \ln Z}{d \ln \beta}, \tag{22}$$

which, using Eq. (4) yields

$$S_T = \frac{\beta \hbar\omega}{e^{\beta\hbar\omega} - 1} - \ln\left(1 - e^{-\beta\hbar\omega}\right). \tag{23}$$

This entropy on the other hand is nothing else but the von Neumann entropy

$$S_T = -\mathrm{Tr}\{\rho \ln \rho\}. \tag{24}$$

As before we can introduce the Rényi–entropy generalization of this quantity the following way,

$$R_q^{(T)} = \frac{1}{1-q} \ln \mathrm{Tr}\{\rho^q\}. \tag{25}$$

With the help of the expression for the partition sum, $Z(\beta\hbar\omega)$, given in Eq. (11), we may obtain the explicit form of these entropies using the following expression

$$I_q^{(T)} = \mathrm{Tr}\{\rho^q\} = \frac{Z(q\beta\hbar\omega)}{Z^q(\beta\hbar\omega)} = 2^{q-1}\frac{\sinh^q(\beta\hbar\omega)}{\sinh(q\beta\hbar\omega/2)} \tag{26}$$

$$R_q^{(T)} = \frac{1}{1-q} \ln I_q^{(T)} \tag{27}$$

In analogy with the phase space distribution, we may also define a thermodynamic measure of the extension of the density operator using

$$D_T^{-1} = \mathrm{Tr}\{\rho^2\}\ , \tag{28}$$

which is a special case of the Rényi entropy with $q = 2$ [(see Eq. (27)], i.e., $R_2^{(T)} = \ln D_T$. For the case of the HO we find

$$D_T = \frac{e^{2\beta\hbar\omega} - 1}{(e^{\beta\hbar\omega} - 1)^2}. \tag{29}$$

The thermodynamic analogue of the structural entropy can also be calculated as

$$S_{str} = S_T - \ln D_T, \tag{30}$$

which for the case of the HO leads to

$$S_{str}^{(T)} = \frac{\beta\hbar\omega}{e^{\beta\hbar\omega} - 1} + \ln\left(\frac{e^{\beta\hbar\omega} - 1}{e^{2\beta\hbar\omega} - 1}\right). \tag{31}$$

Clearly this expression has a limit of Eq. (21) for $\beta\hbar\omega \to 0$, i.e. in the classical limit we do get the desired and expected value. The T/T_0 dependence of S_T (Eq. (23)), $R_2^{(T)} = \ln D_T$ (Eq. (29)), S_{str}^T (Eq. (31)) together with I_W (Eq. (16)) are given in Fig. (1). Notice the cross-over regime in the behavior of S_{str}^T of the low temperature limit, vanishing complexity and large temperature limit of the complexity of the Husimi function represented by a Gaussian over the two-dimensional phase space, see Eq. (21). The $\beta\hbar\omega \to 0$ limit, as it should, shows the classical behavior.

For completeness using the expression of the partition sum, Eq. (11), we give the expressions for the free energy, F, the mean energy, U, and the specific heat, C_V. The respective quantities read [34]

$$F = -\frac{1}{\beta}\ln Z(\beta) = \frac{1}{\beta}\ln\left(e^{\beta\hbar\omega} - 1\right) - \frac{\hbar\omega}{2}, \tag{32}$$

$$U = F + \beta\frac{\partial F}{\partial\beta} = \frac{\hbar\omega}{2}\frac{e^{\beta\hbar\omega} + 1}{e^{\beta\hbar\omega} - 1}, \tag{33}$$

$$C_V = -\beta^2\frac{\partial U}{\partial\beta} = \frac{(\beta\hbar\omega)^2 e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega} - 1)^2}. \tag{34}$$

These functions are depicted in Fig. (2) as a function of T/T_0, where $T_0 = \hbar\omega/k_B$. Again the respective low- and high temperature limits provide the expected behavior for thermodynamic functions, e.g. the free energy, the mean energy, the specific heat and the entropy.

4 Uncertainty at finite temperature

The application of Husimi distributions already involves an inherent use of Heisenberg's uncertainty principle through the gaussian broadenings in both, x and p-directions. The size of the Husimi distribution over the phase space is then calculated as

$$\Delta_H = (\Delta X)_H(\Delta P)_H. \tag{35}$$

This quantity can be calculated using the variances over coordinate and momentum, which therefore are expected to give a generalized uncertainty relation valid for finite temperature, β. Furthermore, as Zurek pointed it out [35, 36], the typical size of the states over the phase space are related to the decoherence properties of the system.

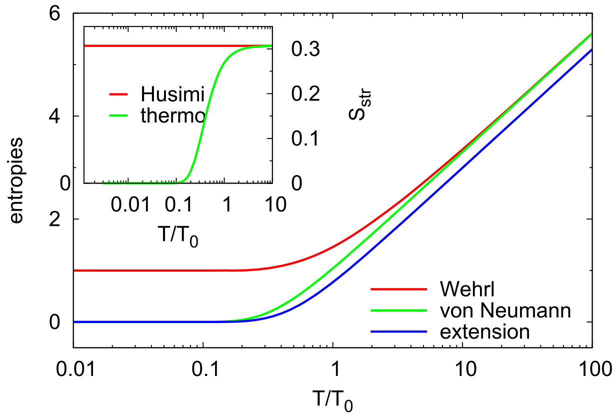

Fig. 1 Several entropies of the density operator vs. T/T_0, where $T_0 = \hbar\omega/k_B$. The inset shows the S_{str} for both the Husimi distribution and that obtained using the density matrix

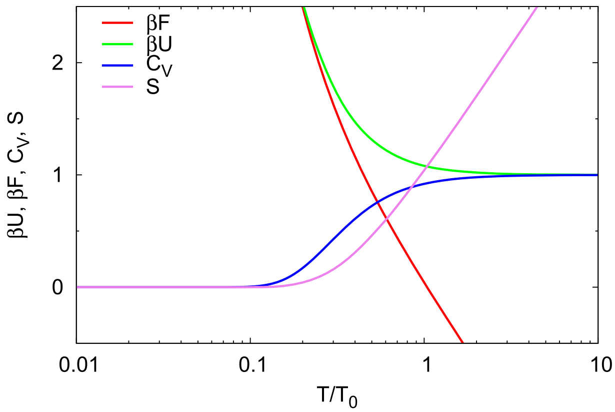

Fig. 2 The mean energy, the free energy, the specific heat, and the entropy vs T for the harmonic oscillator in units of $T_0 = \hbar\omega/k_B$

Let us define the variances of the phase space distribution over coordinate and momentum since both $\langle x\rangle_H$ and $\langle p\rangle_H$ vanish

$$\langle x^2\rangle_H = \int dx\, x^2 \rho(x, p) = \frac{2}{1 - e^{-\beta\hbar\omega}}\sigma_x^2 \tag{36}$$

and

$$\langle p^2\rangle_H = \int \frac{dp}{2\pi\hbar}\, p^2 \rho(x, p) = \frac{2}{1 - e^{-\beta\hbar\omega}}\sigma_p^2, \tag{37}$$

where σ_x and σ_p are the broadenings due to the coherent state representation with $\sigma_x\sigma_p = \hbar$. Therefore we obtain using Eq. (15),

$$\Delta_H = D_H \frac{\hbar}{2} \tag{38}$$

Clearly the low temperature limit, $\beta \to \infty$, yields the lowest value for $\Delta_H = \hbar$ since then $D_H \to 2$. The minimum is twice as much as the usual $\hbar/2$ because the uncertainty due to the state and that of the Husimi function add up equal contributions of $\hbar/2$. The high temperature limit, on the other hand, shows a divergent uncertainty that is in accord with the expectations.

The virial theorem also relates the mean energy (33) to both $\langle x^2 \rangle$ and $\langle p^2 \rangle$ with $U = m\omega^2 \langle x^2 \rangle$ and $U = \langle p^2 \rangle / (2m)$. Hence we easily obtain

$$\langle x^2 \rangle = \sigma_x^2 \frac{e^{\beta\hbar\omega} + 1}{e^{\beta\hbar\omega} - 1}, \tag{39}$$

and

$$\langle p^2 \rangle = \sigma_p^2 \frac{e^{\beta\hbar\omega} + 1}{e^{\beta\hbar\omega} - 1}, \tag{40}$$

which, using Eqs. (36) and (37), are directly linked with the corresponding phase space values as

$$\langle x^2 \rangle_H = \frac{2}{1 + e^{-\beta\hbar\omega}} \langle x^2 \rangle \tag{41}$$

and

$$\langle p^2 \rangle_H = \frac{2}{1 + e^{-\beta\hbar\omega}} \langle p^2 \rangle, \tag{42}$$

and hence we obtain

$$\Delta x \Delta p = (D_H - 1) \frac{\hbar}{2}. \tag{43}$$

The latter expression shows that in the quantum limit of $\beta \to \infty$ $D_H \to 2$ therefore the expected minimum uncertainty is obtained in this limit. On the other hand for large enough temperature the phase space and quantum uncertainties equal and they are large.

Finally let us discuss the rate at which this system is capable to decohere. The parameter describing this situation has been introduced by Zurek [35, 36]

$$\alpha = \frac{\hbar}{\Delta_H}. \tag{44}$$

In Fig. 3 the behavior of α is shown as a function of T/T_0 where $T_0 = \hbar\omega/k_B$. For low enough temperatures the parameter remains constantly unity keeping coherent system but as it decreases decoherence occurs more probably. It is remarkable that at $T = T_0$, i.e. when $\beta\hbar\omega = 1$, the decoherence is already substantial, $\alpha \approx 0.632$.

5 Conclusions

In this paper we have analyzed the characterization of quantum states using generalized entropies. We have shown that the appropriate low-T and high-T limits naturally follow in the case of using Rényi-entropies. Especially the so-called structural entropy being defined as the difference between two prominent Rényi entropies provides more

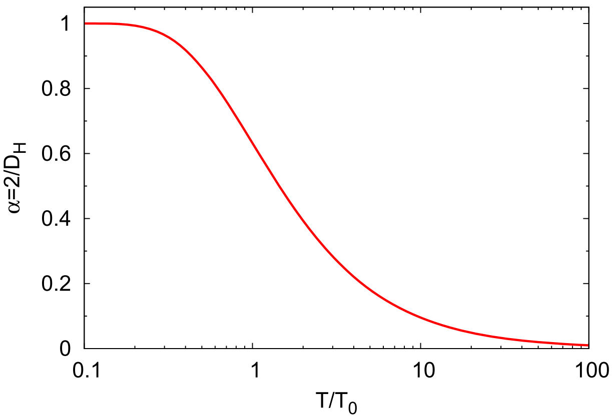

Fig. 3 The decoherence parameter introduced by Zurek

detailed behavior in the correspondence between the quantum and classical pictures. In fact it is able to mark the cross-over region quantum and classical as a function of the parameter $\hbar\omega/k_B T$. As the structural entropy happens to be in direct relation with the so-called LMC complexity measure, we can trace the complexity properties of quantum and classical descriptions.

Furthermore, as a byproduct, it is shown that the space extension of the Husimi function of a quantum state is shown to obey a temperature dependent uncertainty principle. Further investigations of quantum systems in phase space representation show a very rich picture that is unaccessible in the marginal, position or momentum space representations. These results will be presented in subsequent publications.

Funding Open access funding provided by Budapest University of Technology and Economics.

References

1. I. Varga, J. Pipek, Phys. Rev. E **68**, 026202 (2003)
2. J. Pipek, I. Varga, Phys. Rev. A **46**, 3148 (1992)
3. J. Pipek, I. Varga, Int. J. Quantum Chem. **51**, 539 (1994)
4. J. Pipek, I. Varga, T. Nagy, Int. J. Quantum Chem. **37**, 529 (1990)
5. J. Pipek, I. Varga, Int. J. Quantum Chem. **64**, 85 (1997)
6. I. Varga, J. Pipek, Phys. Rev. B **42**, 5335 (1990)
7. I. Varga, J. Pipek, B. Vasvári, Phys. Rev. B **46**, 4978 (1992)
8. I. Varga, J. Pipek, J. Phys.: Condens. Matter **6**, L115 (1994)
9. I. Varga, J. Pipek, J. Phys.: Condens. Matter **10**, 305 (1998)

10. I. Varga, E. Hofstetter, M. Schreiber, J. Pipek, Phys. Rev. B **52**, 7783 (1995)
11. I. Varga, Y. Ono, T. Ohtsuki, J. Pipek, Phys. Status Solidi B **205**, 373 (1998)
12. M. Metzler, I. Varga, J. Phys. Soc. Jpn. **67**, 1856 (1998)
13. I. Varga, E. Hofstetter, J. Pipek, Phys. Rev. Lett. **82**, 4683 (1999)
14. J. Pipek, I. Varga, E. Hofstetter, Physica E **9**, 380 (2001)
15. P. Marcus et al., Phys. Rev. B **104**, 184204 (2021)
16. B. Sziová, S. Nagy, Z. Fazekas, Entropy **23**(8), 936 (2021)
17. S. Nagy et al., *Computational Intelligence and Mathematics for Tackling Complex Problems 3* (Springer, Cham, 2022), p. 111
18. R. López-Ruiz, H.L. Mancini, X. Calbet, Phys. Lett. A **209**, 321 (1995)
19. K.D. Sen (ed.), *Statistical Complexity, Applications in Electronic Structure* (Springer, Berlin, 2011)
20. R. López-Ruiz, Biophys. Chem. **115**, 215 (2005)
21. A. Rényi, Rev. Int. Stat. Inst. **33**, 1 (1965)
22. F. Pennini, A. Plastino, Phys. Lett. A **374**, 1927 (2010)
23. F. Pennini, A. Plastino, G.L. Ferri, F. Olivares, Phys. Lett. A **372**, 4870 (2008)
24. F. Pennini, A. Plastino, Phys. Lett. A **381**, 212 (2017)
25. R. Branada, F. Pennini, A. Plastino, Phys. A **511**, 18 (2018)
26. K.E. Cahill, R.J. Glauber, Phys. Rev. **177**, 1882 (1969)
27. K. Husimi, Proc. Phys. Math. Soc. Jpn. **22**, 264 (1940)
28. D. Gabor, J. Inst. Electr. Eng., Part 1 **93**, 429 (1946)
29. M.O. Scully, M.S. Zubairy, *Quantum Optics* (Cambridge University Press, Cambridge, 1997)
30. W.P. Schleich, *Quantum Optics in Phase Space* (Wiley VCH-Verlag, Berlin, 2001)
31. A. Wehrl, Rev. Mod. Phys. **50**, 221 (1978)
32. E.H. Lieb, Commun. Math. Phys. **62**, 35 (1978)
33. E.P. Wigner, Phys. Rev. **40**, 749 (1932)
34. R.K. Pathria, *Statistical Mechanics*, 2nd edn. (Butterworth-Heinemann, Oxford, 1996)
35. W.H. Zurek, Nature **412**, 712 (2001)
36. W.H. Zurek, Phys. Today **44**, 36 (1991)