Quantum Phase Transitions in Phase Space

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We apply the Wigner function formalism from quantum optics, through Wootters’ discrete Wigner function, to detect quantum phase transitions in critical spin-½ systems. We develop a general formula relating the discrete Wigner function and the thermodynamical quantities of spin models, which allows us to introduce a novel way to represent, detect, and distinguish first-, second- and infinite-order quantum phase transitions in phase space. We establish that the discrete Wigner function provides a simple, experimentally promising tool in the study of many-body systems and we show its relation with measures of quantum correlations.

Introduction.– The use of quantum information tools in understanding many-body quantum systems continues to be a fertile line of research [1–3]. In particular, the use of entanglement and more general forms of quantum correlation, i.e. quantum discord and coherence, to spotlight quantum phase transitions (QPTs) and extract their critical exponents has cemented the important role that such figures of merit play in unraveling the curious properties of many-body systems [4–24]. Indeed, while QPTs only strictly occur at zero-temperature, approaches based on these quantum information theoretic tools have revealed that signatures of these phenomena persist even at finite temperatures and can be rigorously studied [1].

From quantum optics, the Wigner function, which is a quasi-probability distribution in phase space, is known to be a valuable tool in assessing the non-classical nature of systems [26, 27]. While originally defined in a continuous variable setting, for systems with discrete spectra, the so-called discrete Wigner function (DWF) can be defined [26–28]. Such semi-classical tools have been shown to be useful in studying the dynamic properties of many-body systems [29–33].

Recently, it has been established that the Wigner function can be used to define a bonafide measure of quantum correlations [34, 35]. Therefore, given the clear relationship between correlation measures and QPTs, it is natural ask is whether the DWF also allows us to pinpoint which combinations of spin-spin correlation functions are relevant for characterizing the critical properties of the systems. Thus, in addition to being a useful tool in the study of QPTs, we establish the DWF also provides insight into why a particular behavior may be observed for a given measure of quantum correlations across a QPT.

To begin we will outline the discrete Wigner function formalism at the basis of our analysis and establish a general formula relating the DWF with quantum spin-½ chains. We then analyze two paradigmatic spin-chains, the Ising model which exhibits a second-order quantum phase transition, and the XXZ model which exhibits a first- and a continuous (or infinite)-order quantum phase transition.

Theory.– The original formulation for the Wigner function provides a phase space representation of quantum states with continuous degrees of freedom [36, 37]. For discrete systems, several methods have been developed to represent a quantum system with a finite dimensional Hilbert space in phase space [38]. Among these techniques, the formalism for the discrete Wigner function (DWF) for systems with exactly N (prime number) orthogonal states developed by Wootters [26, 27] provides arguably the most natural candidate for our purposes. For such systems the phase space is an N×N grid, labelled by a pair of coordinates (x, p), each taking values from 0 to N − 1 and for each coordinate we define the usual addition and multiplication mod N. If the dimension of the system is N = m^k, with m a prime and k an integer greater than 1, the phase space is constructed by performing the k-fold Cartesian product of m×m phase spaces. Naturally, the simplest example one can consider is a system with two orthogonal states, i.e. a qubit with N = 2, whose discrete phase space consists of four points, while for a composite system of two qubits, i.e. N = 2^2, which will be the focus of this work, the phase space is formed by 16 points, cf. Table I. Each point in the phase space is described by the discrete phase point operator ˆA(x, p). For a single qubit it is given by

$$\hat{A}(x_1, p_1) = \frac{1}{2}(\hat{1} + (-1)^{i_1} \sigma^x + (-1)^{p_1} \sigma^y + (-1)^{i_1+p_1} \sigma^z),$$

(1)

where σ^i (i = x, y, z) are the usual Pauli operators. For composite systems the phase point operators are constructed from the tensor product of the phase point operators of the corresponding subsystems, i.e. $\hat{A}(x_1, p_1) \otimes \hat{A}(x_2, p_2) \otimes \cdots \otimes \hat{A}(x_k, p_k).$ Since the $\hat{A}(x, p)$’s form a complete orthogonal basis of the Hermitian N×N matrices, any density matrix can be decomposed as $\rho = \sum_{(x, p)} W(x, p) \hat{A}(x, p),$ where the real-valued coefficients

$$W(x, p) = \frac{1}{N} \text{Tr}(\rho \hat{A}(x, p)),$$

(2)

correspond to the DWF and N is the dimension of the overall system.
TABLE I: Discrete phase space for (a) one qubit and (b) two qubits

(a) One qubit

| 0 | 1 |
|---|---|
| 0 | p₁ |
| 1 |  |
| x₁ |

(b) Two qubits

| 00 | 01 | 10 | 11 |
|----|----|----|----|
| 00 | 01 | 10 | 11 |
| p₁ | p₂ |

In what follows ρ will be the reduced density matrix for two sites i and j with i < j, separated by some lattice spacing m = j − i, of an infinite quantum spin-½ chain, which can be expressed as

$$\rho_{i+m} = \frac{1}{4} \sum_{αβ=0}^{3} p_{αβ} σ_α^i ∘ σ_β^m, \quad (3)$$

where \( p_{αβ} = ⟨σ_α^i σ_β^m⟩ \) are the spin-spin correlation functions, \( (α, β) = 0, x, y, z \). Substituting Eq. (1) and (3) into (2), and using the \( Z_2 \) symmetry of quantum spin-½ models that we will consider, after some manipulation we find

\[
W(x_1, x_2; p_1, p_2) = \frac{1}{16} \left( 1 + (-1)^{x_1} + (-1)^{x_2} \right) (σ^2) \\
+ (-1)^{p_1+p_2} (σ_1^x σ_1^x) + (-1)^{x_1+x_2} (σ_1^x σ_2^x) \\
+ (-1)^{x_1+x_2+p_1+p_2} (σ_1^x σ_2^x) \quad (4)
\]

This expression is central to our analysis. On inspection it is evident that the DWF for a given choice of \((x_1, x_2)\) involves contributions from the various spin-spin correlation functions as well as the magnetization, which are central to spotlighting critical behavior. An advantage of Eq. (4) is that it allows for a panoramic view of the properties of the system. In particular, evaluating the various DWF allows to focus in on which contributions are relevant in exhibiting the critical behavior. Since a given correlation measure will often depend on only specific spin-spin correlation functions, evaluating Eq. (4) also allows a window into understanding the behavior of measures of quantum correlations across QPTs. A further advantage of Eq. (4) is that any given DWF is comparably easy to access experimentally, at variance with some correlation measures that can require full quantum state tomography. We remark that this expression is not specific to the models considered in this work, but applies to any Hamiltonian that is real and exhibits \( Z_2 \) symmetry.

**Discrete Wigner functions and equilibrium quantum phase transitions.**—We begin by applying the DWF approach to the paradigmatic 1D transverse Ising model with periodic boundary conditions

$$\mathcal{H}_{\text{Ising}} = -\sum_{i=0}^{N-1} (Jσ_i^x σ_{i+1}^x + Bσ_i^z), \quad (5)$$

where \( J \) is the coupling strength and \( B \) the transverse magnetic field strength. Setting \( λ = J/B \), in the thermodynamic limit this model exhibits a ferro- to para-magnetic second order quantum phase transition (2QPT) at the critical point \( λ_c = 1 \). It is well known that various measures of quantum correlation accurately pinpoint this QPT \([4, 5, 7–11, 13]\), and therefore since the DWF is constructed from combinations of correlation functions that enter into the definition of such measures, it is not surprising that we find a qualitatively similar behavior. In line with these previous studies, Fig. 1 and Table II show the first derivative of the DWFs for a nearest neighbor pair of spins. We see that there are six characteristic behaviors and all of them clearly signal the 2QPT by showing a divergence in the first derivative at the critical point. The advantage of the DWF is that is can provide more information about which quantities are playing an important role in dictating the properties of the system. For the Ising case, as all discrete phase space points exhibit a qualitatively similar behavior, choosing to study any one in particular is sufficient to study the QPT. Since a given correlation measure will be expressible in terms of the discrete phase space elements, all of which are sensitive to the 2QPT, it is clear that any such measure will then be equally sufficient in revealing the critical properties of the system. We remark, while here we have only reported the behavior for nearest neighbor pairs, qualitatively similar results hold for arbitrarily long-range pairs. As we will see, the fact that all DWF behave qualitatively the same is a feature particular to the Ising model. The advantage of studying the DWF becomes more apparent when we turn our attention to systems with richer phase diagrams.

To this end we consider the XXZ model with periodic
where $\Delta$ is the anisotropy parameter. The phase diagram is split into three regions, separated by two different QPTs. For $\Delta \leq -1$, the system is in a ferromagnetic (gapped) phase and at $\Delta = -1$ a first-order quantum phase transition (1QPT) occurs. For $-1 < \Delta < 1$, the system is in a gapless (Luttinger liquid) phase and at $\Delta = 1$ an infinite-order continuous quantum phase transition (CQPT) occurs, known as the Kosterlitz-Thouless QPT [39]. Finally, for $\Delta > 1$, the system enters the anti-ferromagnetic (gapped) phase. The equilibrium properties of this model have been well studied, and in particular various measures of quantum correlations and their behavior across the different QPTs have been explored [7, 9, 21–23].

While entanglement and quantum discord were shown to reveal the critical points, their qualitative behaviors were shown to be strikingly different [9]. Here, by examining the DWF we can shed greater light on these behaviors and show that when extremization procedures are employed, features spotlighting criticality become more pronounced.

Fig 2 and Table III shows the three different representative behaviors for the DWF, Eq. (4), for the XXZ chain as a function of $\Delta$, and their corresponding first and second derivatives for nearest-neighboring sites. Let us first consider the behavior of the DWF at the corners of the discrete phase space i.e. (00,00), (00,11), (11,00) and (11,11) [cf. Fig. 2 (a)]. We see the DWF is discontinuous at the 1QPT $\Delta = -1$ while it reaches a minimum at the CQPT at $\Delta = 1$, after which the DWF approaches zero with increasing the anisotropy. This behavior is qualitatively similar to that of the entanglement measured via concurrence, shown in Fig. 3 (b). The relation between the behavior of the DWF in these four points and that of the concurrence becomes apparent when we examine which terms in Eq. (4) contribute to the DWF compared with those that enter into the expression for the entanglement. The concurrence is simply $2\langle \sigma^z_1 \sigma^z_2 \rangle$, while the DWF at these points depends on both $\langle \sigma^x_1 \sigma^x_2 \rangle$ and $\langle \sigma^y_1 \sigma^y_2 \rangle$. It is interesting that we see here the negativity of the DWF coincides with the presence of entanglement in the state, inline with a negative behavior of the continuous Wigner function implying genuine non-classicality of the state [34, 35].

The second significant behavior is located at phase space points (00,01), (00,10), (11,01), and (11,10) shown in Fig. 2 (b) where, at variance with the previous cases, signatures of the critical points are less immediately evident in the behavior of the DWF. For $\Delta < -1$ these functions are constant and exhibit a change at the 1QPT, which is clearly shown by computing their derivative with respect to $\Delta$. On inspection we can see a point of inflection around $\Delta = 1.5$. Looking at the first derivative of the DWF we see that it presents an amplitude bump at $\Delta = 1.5$, and the second derivative is divergent at $\Delta = -1$ and around $\Delta = 1$. The more peculiar behavior seen in these DWF is due to the destructive interference at these phase space points between the two terms that control the DWF which are $1 + \langle \sigma^x_1 \sigma^x_2 \rangle$ and $-2\langle \sigma^y_1 \sigma^y_2 \rangle$, and the inflection point seen arises from a sudden change in the concavity of $-2\langle \sigma^y_1 \sigma^y_2 \rangle$. Thus, unlike in the Ising model where all DWFs readily witness the 2QPT, the DWF in these four points can only easily signal the 1QPT exactly, while for the CQPT it shows only some anomalies around $\Delta = 1$. However, we will revisit this behavior in the context of extremization procedures shortly.

Finally we consider the remaining eight phase space points, Fig. 2 (c). Here the DWF depends solely on a single term, $1 - \langle \sigma^z_1 \sigma^z_2 \rangle$, and owing to the fact that spin-spin correlation functions are discontinuous at $\Delta = -1$ and that on their own they fail at revealing the CQPT at $\Delta = 1$ the DWF at these points inherits these properties from the $\langle \sigma^z_1 \sigma^z_2 \rangle$ contribution.
which explains why the DWF is discontinuous and its derivatives are divergent at $\Delta = -1$, while it does not show any special behavior at $\Delta = 1$.

Minimization and maximization of the discrete Wigner function. We have seen that the discrete phase space of the XXZ model is dominated only by three characteristic behaviors of the DWF. Given the relationship between various phase-space points and correlation measures, we consider the minimization and maximization of the DWF in phase space. Such a procedure is often involved in measures of quantum correlations such as quantum discord. Often these correlation measures stand out as the preferred figures of merit for studying criticality [8–11, 40]. Let $W_M$ and $W_m$ be the maximized and minimized DWF over the discrete phase space, respectively, given by

$$W_M = \max(W_{00,00}, W_{00,01}, W_{01,00}),$$

$$W_m = \min(W_{00,00}, W_{00,01}, W_{01,00}),$$

(7)

where we have chosen $W_{00,00}$, $W_{00,01}$, and $W_{01,00}$ to capture the three distinct behaviors exhibited in the discrete phase space.

In Fig. 3 (a) we see $W_M$ reveals a cusp exactly at the CQPT and thus its first (second) derivative is discontinuous (divergent) at the critical point, $\Delta = 1$, as shown in the inset. This indicates that the DWF could be a good alternative to correlation measures that involve extremization procedures due to the comparative simplicity in its calculation and its easy physical interpretation following Eq. (4). Moreover, the behavior of $W_m$, depicted in Fig. 3 (a) is qualitatively identical to that of the entanglement [panel (b)]. Again we see under minimization, negativity of the DWF again coincides with the establishment entanglement.

Beyond the comparative simplicity in its calculation, an advantageous aspect of the phase space technique presented here is the panoramic view of the different possible states of a quantum system, which offers a novel perspective for examining QPTs, particularly the CQPT. Looking at $\partial^2 W_M$ of the DWF in the inset of Fig. 3 (a) and the corresponding second derivatives of the distinct behaviors in discrete phase space shown in Fig. 2, where we have destructive interference between the terms that control the DWF (for example the point $(00,01)$), we find that both behave quite similarly. Therefore, we argue that to be able to detect reliably the CQPT, one requires a figure of merit that includes all the spin-spin correlation functions of the quantum system. This is further evidenced by the fact that the other parts of the phase space, where only a single spin-spin correlation term is dominant, are less sensitive to this QPT.

Conclusions. We have presented an alternative method to study quantum phase transitions from a phase space perspective using the discrete Wigner function (DWF). By establishing a connection between the DWF and the thermodynamical quantities of a quantum spin-$\frac{1}{2}$ chain, we have shown the DWF to be a versatile tool in studying first-, second-, and infinite-order quantum phase transitions. In addition, this approach may provide a promising tool for the experimental investigation of quantum phase transitions following the procedures proposed in Refs. [41, 42]. Furthermore, through Eq. (4), a given DWF is easily physically interpreted. Beyond characterizing phase transitions, our approach also provides insight into the behavior of various correlation measures in such systems, in particular we have shown that the representation of quantum spin-$\frac{1}{2}$ chain in the discrete phase space underlies the entanglement. While we have focused on equilibrium systems, we expect our approach to be useful in examining the dynamical properties of such critical systems [29–33, 43, 44]. We also expect the DWF approach used here can be readily extended to multipartite systems, and thus may provide an avenue to understand the role of many-body correlations at quantum phase transitions [15–19].

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