Thermodynamical Versus Optical Complementarity

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We establish correspondence between macroscopic thermodynamical quantities and complementarity in wave interference. The well known visibility and predictability in a double slit–like experiment are shown to be connected to magnetic susceptibility and magnetization of a general interacting spin chain. This gives us the ability to analyze the tradeoff between thermodynamical quantities in the same way that we understand the tradeoff between interference fringes and the “visibility” in an interferometer.

We thus obtain new physical insights into usually complicated thermodynamical models, such as viewing a phase transition simply as a change from an effective single slit diffraction to a double slit interference. PACS-Numbers: 42.25Hz, 05.70.-a, 05.30.d

Introduction. Spin chains have been analyzed within many contexts in the last hundred years of physics. They frequently provide very precise models for solids within which one can study their various macroscopic properties. Typically one studies the response of solids to different external conditions, such as the changing magnetic field, temperature etc. The standard approach is first to construct the Hamiltonian for the chain, which is then diagonalized through a sequence of transformations. The resulting eigenvalues are then used to obtain the partition function and from that all macroscopic quantities can in principle be derived.

It frequently happens that the diagonalizing method involves highly complicated transformations which do not reveal much physics, and ultimately leave very little trace in the final quantities such as the heat capacity or magnetic susceptibility. Physicists are not really interested in the details of diagonalization, but in the relationship between various macroscopic quantities, any tradeoff between them and any limitation in the information we can have about them. Diagonalization procedure itself, however, throws very little light on these issues. Partition functions, in particular, do not by themselves reveal much about the relationships between derived macroscopic quantities.

The main purpose of this Letter is to further our understanding of thermodynamical quantities by making an analogy between optical interference phenomena and the summation of the exponential Boltzmann energy factors in the partition function (of spin lattice). As we will show this analogy helps us to clarify relationships and tradeoffs between thermodynamical quantities such as magnetization and magnetic susceptibility in the same way that we understand the tradeoff between the interference fringes and the “which–path” information in an interferometer. Our work is also inspired by the analogy between Feynman’s quantum mechanical propagator and the thermodynamical partition function [1].

The Letter is organized as follows. We first describe complementarity in a double slit experiment between the “predictability” of the wave/particle going through one of the slits and the “visibility” of the interference fringes. Predictability and visibility, which will be formally quantified below, will be our pair of complementary properties, so that the better we know one of them, the less we can determine the other one. We will then discuss the correspondence between double slit interference and the thermodynamical partition function for a chain of non-interacting two level systems. From that we will argue that there is a thermodynamical analogue to the dynamical double slit complementarity. This thermodynamical complementarity is seen in a tradeoff relationship between quantities such as the magnetization of a system and its susceptibility. Roughly speaking, the higher the value of one of them, the lower will be the value of the other one, in direct analogy with predictability and visibility. We show that this is a general result that applies to more complicated interacting spin chains and allows us to understand phase transitions in the same spirit.

Complementarity in double slit experiments. The concept of duality in interferometric or double slit–like devices is the basic ingredient of any physical theory of waves. It is also at the heart of the quantum mechanical wave–particle duality, since in quantum theory waves are used to describe matter as well. For simplicity, we will use the quantum language to discuss interference, however, the whole analysis applies to any (classical or quantum) wave theory. The qualitative statement that “the observation of an interference pattern and the acquisition of which–way information are mutually exclusive” has only recently been rephrased as a quantitative statement [2]:

\[ P^2(y) + V_0^2(y) \leq 1. \]  

(1)

where the equal sign is only valid for pure states. \( V_0 \) is the fringe visibility which quantifies the sharpness or contrast of the interference pattern (“the wave–like property”), whereas \( P \) denotes the the path predictability, i.e., the \( a \)\textit{ priori} knowledge one can have on the path taken by the interfering system (“the particle–like property”). Since we restrict our analysis to two-path interferometry, the
predictability is defined by
\[ P = |p_I - p_{II}|, \]
where \( p_I \) and \( p_{II} \) are the probabilities for taking each path \((p_I + p_{II} = 1)\). Usually these quantities depend on one external parameter which we label by \( y \). For example, consider the double slit experiment for which the intensity is given by
\[ I(y) = F(y) \left(1 + V_0(y) \cos(\phi(y))\right), \]
where \( F(y) \) is specific for each setup and \( \phi(y) \) is the phase-difference between the two paths. The variable \( y \) characterizes in this case the detector position. Note that this formalism applies to many different physical situations. In Ref. [8] the authors investigated physical situations for which the expressions of \( V_0(y) \), \( P(y) \) and \( \phi(y) \) can be analytically computed, i.e. they depend only linearly on the variable \( y \). This included interference patterns of various types of double slit experiments (\( y \) is linked to position), but also oscillations due to particle mixing \((y \) is linked to time), e.g. by the neutral kaon system, and also Mott scattering experiments of identical particles or nuclei \((y \) is linked to a scattering angle). All these two-state systems belonging to distinct fields of physics can then be treated via the generalized complementarity relation in a unified way.

**Thermodynamical complementarity.** We first illustrate with a simple example how complementary manifests itself in thermodynamical systems. Suppose that we have an ensemble of \( N \) two-level non-interacting systems, with eigenvalues \( E_1 = E \) and \( E_2 = -E \). Then the partition function is
\[ Z = (e^{-E/kT} + e^{E/kT})^N = 2^N \cosh N \frac{E}{kT}. \]
This contains all thermodynamical information one can extract from the system. Let us first write down the free energy as
\[ F = -kT \ln Z = -kTN \ln(2 \cosh \frac{E}{kT}). \]
Suppose that this describes \( N \) spins in an external magnetic field in which case the energy is proportional to the magnetic field \( B \), like so \( E = \mu B \). Now, the magnetization and the susceptibility are given by:
\[ M = \frac{\partial F}{\partial B} = 2\mu N \tanh \frac{E}{kT}, \]
\[ \chi = \frac{\partial^2 F}{\partial B^2} = 2\mu^2 N \cosh^{-2} \frac{E}{kT}. \]
The crux of our analogy is that \( M \) and \( \chi \) behave like the predictability and the visibility. More precisely, one immediately derives from Eq. \[5\] and Eq. \[6\] that the following equation has to hold
\[ \left(\frac{M}{2\mu N}\right)^2 + 2kT \frac{\chi}{4\mu^2 N} = 1. \]
There is a tradeoff between magnetization and susceptibility (per spin) at a fixed temperature: the larger one of the quantities, the smaller the other one and vice versa. Physically, this is to be expected, since higher magnetization implies a better knowledge of the spin direction and, in turn, that different spins are less correlated (in the statistical sense); hence susceptibility is smaller.

In order to compare this with the wave complementarity (both classical and quantum), we now discuss interference pattern from two slits, whose amplitude transmission function is a Gaussian. The intensity is given by
\[ I(y) \propto e^{-(y-d/2)^2/2\sigma^2} + e^{-(y+d/2)^2/2\sigma^2} e^{i\phi(y)} \]
\[ = e^{-(y^2 + d^2/4)/\sigma^2} 2 \cosh(yd/\sigma^2) \left( 1 + \frac{\cos \phi(y)}{\cosh(yd/\sigma^2)} \right) \]
where \( d \) is the separation of the slits, \( \sigma \) is the effective width of the amplitude transmission function and \( \phi(y) \) is the phase arising from the path difference. From this formula we can infer that the visibility is given by
\[ V_0(y) = \frac{1}{\cosh(yd/\sigma^2)}. \]
The predictability can likewise be derived:
\[ P(y) = \left|\tan(yd/\sigma^2)\right|, \]
which obviously fulfills the complementarity relation \[11\] for all \( y \) with the equality sign. We can see that the predictability has exactly the same functional behavior as the magnetization (per spin) in Eq. \[5\]. The susceptibility in Eq. \[6\], on the other hand, behaves in the same way as the visibility. Pushing this analogy one step further, we can identify the energy of the spins with the position variable in the double slit experiment and likewise the inverse of the Boltzmann constant \( k \) with the slit separation \( d \). In this case, the temperature \( T \) corresponds to the effective slit width \( \sigma^2 \) and the energy \( E \) would be the detector position \( y \). For fixed energy, if the temperature is low (corresponding to a narrow slit), the visibility goes to zero, and so (from the existing complementarity) the predictability achieves the maximum value of one. We can also make a different correspondence altogether that will be useful in our interferometric understanding of the phase transition. The ratio of spin energy to temperature \( E/T \) could correspond to the detector position \( y \), while \( 1/k \) is the ratio \( d/\sigma^2 \).

**General Relationship.** We can formalize the tradeoff between the thermodynamical quantities such as the (normalized) magnetization and susceptibility as well as the optical quantities such as the predictability and visibility. A general way of phrasing the complementarity between these is to say that we have a function \( f \) bounded between \(-1 \) and \( 1 \) and we compare its square with its derivative, \( f' \). More precisely, we would like to know for what functions \( f \) do we have that
\[ f^2(x/\alpha) + \alpha f'(x/\alpha) = \beta \]
The shown to exist in well known lattice models. Examples of these more general forms are now extensively used in many situations and has been analyzed by the Boltzmann constant $k$ in the partition function and the effective slit width is given by the Boltzmann constant $k$ divided by the coupling $J$. The thermodynamical limit is obtained by making the array continuous in which case the only surviving interference is between the upper and lower path (all other cross terms cancel). This then reproduces the integral in Eq. (12). In one analogy different detector positions at the screen correspond to different reciprocal temperatures. Therefore if the temperature is high, we have the central maximum of the interference pattern where both of the paths contribute equally (thermodynamically this means that both Boltzmann factors are equal). Remarkably, interference of Boltzmann factors may exist even at zero temperature, and this then signifies the point of quantum phase transition as explained in more detail in the text.

Where for our physical applications $\alpha$ and $\beta$ are non-negative constants. The most general solution is $f(x/\alpha) = \sqrt{\beta} \tanh(\sqrt{\beta}(x/\alpha + c))$, where $c$ is another constant. We can see that the most general solution of the above equation has the form of predictability of Gaussians, or, alternatively, it has the form of a derivative of partition function for a two level system. In the optical case, the predictability is just the difference between the mod squares of the two amplitudes for each slit. Since each amplitude is a Gaussian, this quantity behaves like the tanh function. In thermodynamics, likewise, the partition function for a two level system is a sum of the exponential Boltzmann factors for the two states which is proportional to cosh. When this is differentiated to obtain the magnetization, this gives us again the tanh function.

Our general complementarity bound is in fact an inequality of the type $f^2(x/\alpha) + \alpha f'(x/\alpha) \leq 1$. Some solutions of this inequality can be constructed from the above equality, but we do not have the most general closed form solution. Examples of these more general forms are now shown to exist in well known lattice models.

The $XY$ Heisenberg Model. This model has been extensively used in many situations and has been analyzed in various regimes. The Hamiltonian is given by:

$$H = -\frac{J}{2} \sum_{i=1}^{N} \sigma_i^x \otimes \sigma_{i+1}^x + \sigma_i^y \otimes \sigma_{i+1}^y - \mu B \sum_{i=1}^{N} \sigma_i^z.$$ 

This Hamiltonian was diagonalized in a sequence of complicated transformations. In the large $N$ limit (which is what we are always interested in when it comes to computing thermodynamical quantities) one derives the following partition function

$$\lim_{N \to \infty} \frac{1}{N} \ln(Z^N) = \frac{1}{\pi} \int_0^{\pi} \ln \cosh(C - 2K \cos(\omega)) d\omega$$

where $K = J/2kT$, $C = \mu B/kT$ and $\omega = 2\pi k/N$ are the frequencies of the Fourier transformed fermionic creation and annihilation operators. The free energy is

$$-\frac{F}{NkT} = \frac{1}{\pi} \int_0^{\pi} \ln 2 \cosh(C - 2K \cos(\omega)) d\omega,$$

and so the magnetization and the susceptibility are:

$$\frac{M}{N\mu} = \frac{1}{\pi} \int_0^{\pi} \tanh(C - 2K \cos(\omega)) d\omega,$$

$$\frac{\chi kT}{\mu^2 N} = \frac{1}{\pi} \int_0^{\pi} \cosh^{-2}(C - 2K \cos(\omega)) d\omega.$$ 

Consequently, we obtain the following complementary relation ($\tilde{C}(\omega) = C - 2K \cos(\omega)$)

$$\left(\frac{M}{N\mu}\right)^2 + \frac{\chi kT}{\mu^2 N} \leq \frac{1}{\pi} \int_0^{\pi} \tanh^2(\tilde{C}(\omega)) + \cosh^{-2}(\tilde{C}(\omega)) d\omega = 1.$$ 

We see that the form of these quantities is now more complicated. For each $\omega$ the visibility is given by a cosh-function corresponding to a double slit experiment, however, the susceptibility per spin, i.e. the measurable quantity, is the sum of all visibilities squared. This we can illustrate by a series of double slits as in Fig.1. We set for simplicity $B = 0$ and interpret the inverse temperature $1/T$ as the detector position and $\frac{B}{T}$ as the constant effective slit width. Each of the double slits in the series gives rise to its own predictability and the total predictability is an integral over all individual ones. The integration is over different slit separations corresponding to the value of $\cos(\omega)$.

Phase transitions. Our correspondence between wave optics and thermodynamics allows us to understand and interpret phase transitions in an elegant and transparent way. Briefly stated, for a phase transition to occur in thermodynamics we need the interference in the corresponding optical setting to appear from a pattern that is otherwise effectively a single slit diffraction. If we never have “interference” between two different Boltzmann contributions then we can conclude there is no
Above the critical external field we have no interference model, we now obtain two different domains of behavior. Contrary to the Ising and susceptibility still satisfy the same complementarity relation of the transverse Ising model depending on the magnetic field for different temperatures (blue ≡ kT small; coupling fixed to J = 3). The quantum phase transition occurs at J = B for low temperature, where the complementarity relation is most interesting because both terms contribute. Away from this point either or both of the complimentary quantities become small.

The partition function has contributions of two eigenvalues \( \lambda_+ \geq \lambda_- \), however, in the large \( N \) limit, only the larger of the two eigenvalues survives:

\[
F = \frac{1}{N} \log(\lambda_+^N + \lambda_-^N) \xrightarrow{N \to \infty} \log \lambda_+ \tag{14}
\]

This model is therefore never a two level system and hence there is no phase transition.

On the other hand, the Ising model where the external field is in the \( x \) instead of the \( z \) direction (a transverse field) behaves very differently. Its free energy is given by:

\[
\frac{-F}{NkT} = \frac{1}{\pi} \int_0^\infty \log(2 \cosh \sqrt{K^2 + C^2 - 2KC \cos \omega})d\omega,
\]

and it has a more complex, nonlinear dependence on \( B \) than previously considered. The derived magnetization and susceptibility still satisfy the same complementarity as can be seen from Fig. 2. Contrary to the Ising model, we now obtain two different domains of behavior. Above the critical external field we have no interference and this corresponds to the disordered phase (the visibility is low). At the point of critical field value, the interference appears and we begin to have an ordered phase (here both predictability and visibility contribute significantly as can be seen in Fig. 2). We stress that this quantum phase transition happens at zero temperature, and so the interference is not simply due to the equality of Boltzmann factors introduced by the high temperatures irrespectively of the energy eigenvalues. The interference at high temperatures does also lead to an increase in visibility, but this has no relation to the phase transition. So, the disorder–order transition represents a change from an effective single slit diffraction to a double slit interference scenario. The relationship between degeneracy and criticality is also important for classical phase transitions as is reviewed in detail in [3], and our analysis can equally well be applied here.

**Conclusions.** By viewing the behavior of complex thermodynamical systems as a double slit interference pattern we can gain various insights into the complicated interplay between macroscopic properties of solids. This analogy allows us to trace this interplay directly back to the exponential factors in the partition function which plays the same role as the amplitude transmission function does in optics (or the density matrix in quantum mechanics). A natural next step would be to explore more dimensional systems and make an analogy with a multi slit diffraction grating. It would be also beneficial to exploit this analogy in the other direction, such as defining the free energy for the optical case.

We believe that our work helps us develop an intuition as to which methods of diagonalization can be successfully applied to which models and why some methods fail for some scenarios. For example, in 1931 Bethe used a complicated procedure (Bethe’s ansatz [3]) to diagonalize the one dimensional Ising model. He concluded his work by saying that the application of the same procedure to the two dimensional model was forthcoming in the next paper. However, this paper never happened. From our analogy we understand now that the one dimensional Ising model exhibits no interference phenomena and is therefore intrinsically simple. The critical behavior existing in the two dimensional model, on the other hand, depends crucially on the interference which cannot be handled through Bethe’s ansatz (it requires a more complicated method invented by Onsager and reviewed in [3]).

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