\( \mathcal{PT} \) Symmetry and the Sign Problem

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Abstract

Generalized \( \mathcal{PT} \) symmetry provides crucial insight into the sign problem for two classes of models. In the case of quantum statistical models at non-zero chemical potential, the free energy density is directly related to the ground state energy of a non-Hermitian, but generalized \( \mathcal{PT} \)-symmetric Hamiltonian. There is a corresponding class of \( \mathcal{PT} \)-symmetric classical statistical mechanics models with non-Hermitian transfer matrices. For both quantum and classical models, the class of models with generalized \( \mathcal{PT} \) symmetry is precisely the class where the complex weight problem can be reduced to real weights, i.e., a sign problem. The spatial two-point functions of such models can exhibit three different behaviors: exponential decay, oscillatory decay, and periodic behavior. The latter two regions are associated with \( \mathcal{PT} \) symmetry breaking, where a Hamiltonian or transfer matrix has complex conjugate pairs of eigenvalues. The transition to a spatially modulated phase is associated with \( \mathcal{PT} \) symmetry breaking of the ground state, and is generically a first-order transition. In the region where \( \mathcal{PT} \) symmetry is unbroken, the sign problem can always be solved in principle. Moreover, there are models with \( \mathcal{PT} \) symmetry which can be simulated for all parameter values, including cases where \( \mathcal{PT} \) symmetry is broken.

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I. THE COMPLEX WEIGHT PROBLEM

The sign problem occurs in many branches of theoretical physics, including particle physics, many-body theory, statistical physics and condensed matter theory. The problem arises when the expected value of an observable is computed as a sum over non-positive weights, and perhaps should be called more generally the complex weight problem. For example, in lattice QCD, the introduction of a non-zero chemical potential makes the quark contribution to the functional determinant complex [1, 2]. Because the powerful simulation techniques of lattice gauge theory rely on a positive weight within the functional integral, progress in simulating QCD at finite density has been meager relative to what has been achieved in other aspects of QCD. Similar problems occur in other areas of physics, such as the Hubbard model away from half-filling [3] and systems with topological charges [4].

We will show that $\mathcal{PT}$ symmetry is a powerful tool for analyzing the sign problem. In particular, $\mathcal{PT}$-symmetric systems are precisely the class of systems where the complex weight problem can be reduced to a sign problem, i.e., positive and negative weights. Furthermore, $\mathcal{PT}$ symmetry provides a natural classification scheme for the oscillatory behaviors observed in correlation functions in liquid and crystalline phases, giving us a simple, unified picture of behavior across many areas of physics. Finally, $\mathcal{PT}$ symmetry gives us important information about the solvability of the sign problem, and a framework for future progress in work on particular systems.

The fundamental importance of $\mathcal{PT}$ symmetry was first pointed out by Bender and Boettcher in their seminal work on quantum-mechanical models [5]. Their work grew out of the observation that the Hamiltonian

$$H = p^2 + igx^3. \quad (1)$$

which arises naturally in the study of the Lee-Yang theory of phase transitions [6–11], has only real eigenvalues. Bender and Boettcher observed that the Hamiltonian $H$, while not Hermitian, is invariant under the simultaneous application of the symmetry operations parity $\mathcal{P}: x \rightarrow -x$ and time reversal $\mathcal{T}: i \rightarrow -i$. This symmetry ensures that all eigenvalues of $H$ are either real or part of a complex pair. The argument is simple: if $H \mid \psi \rangle = E \mid \psi \rangle$ then $H \mathcal{PT} \mid \psi \rangle = \mathcal{PT} H \mid \psi \rangle = \mathcal{PT} E \mid \psi \rangle = E^* \mathcal{PT} \mid \psi \rangle$. Thus if $E$ is an eigenvalue, $E^*$ is an eigenvalue as well.
II. QUANTUM MANY-BODY THEORY AND $\mathcal{PT}$ SYMMETRY

We will now show that all quantum many-body problems involving a non-zero chemical potential may be described in terms of a non-Hermitian Hamiltonian with generalized $\mathcal{PT}$ symmetry. We start from a theory with a Hermitian Hamiltonian $H$ and a conserved global quantum number $N$, obtained from a conserved current $j_\mu$, that commutes with $H$. We assume that $H$ is Hermitian and invariant under the combined action of time reversal $T$ and a charge conjugation $C$ that reverses the sign of $j^\mu$. We take the number of spatial dimensions to be $d - 1$, and the spatial volume to be $L^{d-1}$. The grand canonical partition function at temperature $T = \beta^{-1}$ and chemical potential $\mu$ is given by $Z = Tr [\exp (-\beta H + \beta \mu N)]$. If $Z$ is written as a Euclidean path integral, the time component of the current $j^0$ will Wick rotate to $ij^d$, while the chemical potential $\mu$ does not change. This leads directly to a non-positive weight in the path integral, and is the origin of the sign problem in finite density calculations: probabilistic methods do not work. The Euclidean space Lagrangian density may be written as $L - i\mu j^d$ where $L$ is the Euclidean Lagrangian for $\mu = 0$; $\mathcal{L} - i\mu j^d$ is complex. The nature of the problem is changed by changing the direction of Euclidean time, so that we are now considering a problem at zero temperature with one compact spatial dimension of circumference $\beta$. Upon returning to Minkowski space, $j^d$ does not rotate. We pick, say, the $1$ direction to be the new time direction and take the new inverse temperature $L$ to satisfy $L \gg \beta$. When $\mu = 0$, the original Hamiltonian is unchanged, but the partition function is now given by

$$Z = Tr \left[ e^{-LH_\beta} \right]$$

(2)

where

$$H_\beta = H - i\mu \int d^{d-1}x j^d.$$  

(3)

The new Hamiltonian $H_\beta$ is non-Hermitian, but possesses a generalized $\mathcal{PT}$ symmetry, where the role of $\mathcal{P}$ is played by the charge conjugation operator $C$ that changes the sign of $j^0$ and $N$. Under the combined action of $CT$, $j^d \rightarrow -j^d$ and $i \rightarrow -i$, leaving the Hamiltonian $H_{PT}$ invariant. If we introduce the operator $H_L = H - \mu N$, we have the relation

$$Z = Tr \left[ e^{-\beta H_L} \right] = Tr \left[ e^{-LH_\beta} \right]$$

(4)

under the space-time transformation that exchanges directions $1$ and $d$. Note that $Z$ is obtained from $H_L$ by a sum over all eigenstates, but is dominated by the ground state of
We have previously given an explicit example of the construction of $H_\beta$ for the case of QCD with static quarks at finite density \[12\]. After the static quarks are integrated out of the functional integral, the effective action has the form

$$S_{\text{eff}} = \int d^4 x \left[ \frac{1}{4g^2} \left( F_{\mu\nu} \right)^2 - h_F \left( e^{\beta\mu} \text{Tr}_F(P) + e^{-\beta\mu} \text{Tr}_F(P+) \right) \right]$$  \hspace{1cm} (5)

where $P$ is the Polyakov loop $P(\vec{x}) = \mathcal{P} \exp \left[ i \int_0^\beta dt A_4(\vec{x}, t) \right]$ and $h_F$ is a known function of the temperature and the quark mass $M$, going to zero as $M$ goes to infinity. In $1 + 1$ dimensions, the solution of this model reduces to solving a $\mathcal{PT}$-symmetric quantum mechanics problem on the gauge group. The Hamiltonian $H_\beta$, obtained from $S_{\text{eff}}$, is

$$H_\beta = \frac{g^2\beta}{2} C_2 - h_F \beta \left[ e^{\beta\mu} \text{Tr}_F(P) + e^{-\beta\mu} \text{Tr}_F(P+) \right]$$  \hspace{1cm} (6)

and acts on the gauge-invariant physical states which are class functions of $P$ obeying $\Psi[P] = \Psi[gPg^+]$. The operator $C_2$ is the quadratic Casimir operator for the gauge group, the Laplace-Beltrami operator on the group manifold. The group characters form an orthonormal basis on the physical Hilbert space: any gauge-invariant state $\Psi$ can be expanded as $\Psi[P] = \sum_R a_R \text{Tr}_R(P)$. The Hamiltonian $H$ is not Hermitian when $\mu \neq 0$, a direct manifestation of the sign problem, but it is $\mathcal{PT}$ symmetric when $\mathcal{P}$ is taken to be the charge conjugation operator $\mathcal{C}$ that changes $A_\mu$ to $-A_\mu$. In figure 1, we show the real part of the eigenvalues of $H_\beta$, measured in units where $g^2\beta/2$ is set to 1. The overall strength of the potential term is set by the dimensionless parameter $2h_F/g^2$. In the upper graph, $2h_F/g^2 = 0.5$, corresponding to antiperiodic boundary conditions for the heavy quarks. Note the formation of a complex conjugate pair of excited state eigenvalues as $\beta\mu$ increases.

It is also of interest to consider the case of periodic boundary conditions for the heavy quarks, corresponding to $h_F < 0$ \[13\]-\[15\]. The lower graph shows the energy eigenvalues for $2h_F/g^2 = -0.5$, where the ground state becomes part of a conjugate pair as $\beta\mu$ increases. The coalescence of real energy eigenvalues into conjugate pairs with degenerate real parts is typical of $\mathcal{PT}$-symmetric systems, and is usually referred to as broken $\mathcal{PT}$ symmetry. Note that this usage is somewhat different from what is meant by broken symmetry in Hermitian models, where only the symmetry of the ground state is considered. Note that for $N \geq 3$, the heavy quark finite density problem of $SU(N)$ gauge theory is in the universality class of the Lee-Yang problem for $Z(N)$ spin systems \[16\].
III. MODELS FROM STATISTICAL MECHANICS

It is therefore not surprising that there is a class of $\mathcal{PT}$-symmetric $Z(N)$ spin models which are closely related. On each lattice site $j$ there is a spin $w_j$, an element of the group $Z(N)$ which may be parametrized as $w_j = \exp(2\pi in_j/N)$ with $n_j \in \{0, 1, \ldots, N - 1\}$ defined modulo $N$ so that 0 and $N$ are identified. We take the operator $\mathcal{P}$ to be charge conjugation, acting as $n_j \rightarrow -n_j$, or equivalently $w_j \rightarrow w_j^\ast$. The operator $\mathcal{T}$ is again complex conjugation.
Figure 2: Phase diagram for the $d=1\ P\mathcal{T}$-symmetric $Z(3)$ spin model in the $h_R - h_I$ plane at $J = 0.2$. The interpretation of regions Ia, Ib, II and III are given in the text.

Although $\mathcal{P}$ and $\mathcal{T}$ have the same effect on the $w_j$'s, one is a linear operator and the other antilinear. We will show below that $\mathcal{P}$ is implemented as a unitary matrix in the transfer matrix formalism. The Hamiltonian $H$ is defined by

$$-\beta H = \sum_{\langle jk \rangle} J \frac{1}{2} (w_j w_k^* + w_k^* w_j) + \sum_j \left[ h_R (w_j + w_j^*) + h_I (w_j - w_j^*) \right]$$

(7)

where $\beta = 1/T$, $J$, $h_R$ and $h_I$ are real and the sum over $\langle jk \rangle$ represents a sum over nearest-neighbor pairs. $H$ is trivially $\mathcal{P}\mathcal{T}$-symmetric. This class of models has complex Boltzmann weights for $N \geq 3$ when $h_I \neq 0$.

We illustrate the rich behavior possible in these models using the case of a $Z(3)$ model in $d = 1$. If $h_I = 0$, then the transfer matrix $T$ is Hermitian. When $h_I \neq 0$, $-\beta H$ is no longer real and $T$ is no longer Hermitian, but is $\mathcal{P}\mathcal{T}$ symmetric. Figure 2 shows the phase
diagram in the $h_R - h_I$ plane for $J = 0.2$. There are four distinct regions. In region Ia, all three eigenvalues of the transfer matrix are real and positive. This region includes the line $h_I = 0$, and has properties similar to those found in the Hermitian case. In region Ib, all of the eigenvalues are real, but at least one of them is negative. In region II, the eigenvalue of $T$ largest in magnitude is real, but the two other eigenvalues form a complex conjugate pair. In region III, the two eigenvalues largest in magnitude form a complex conjugate pair, and the third, smaller, eigenvalue is real. In both region II and region III, $\mathcal{PT}$ symmetry is broken, but in different ways. Borrowing the terminology from $\mathcal{PT}$-symmetric quantum mechanics, we will describe the behavior in region III as $\mathcal{PT}$-symmetry breaking of the ground state, while region II is $\mathcal{PT}$-symmetry breaking of an excited state. The behavior of the two-point function $G(|j - k|) = \langle w(j) w^\dagger(k) \rangle$ differs substantially in the three regions. In region I, the two-point function falls off exponentially. We show typical behavior in region Ia in figure 3 for point A where $(h_R, h_I) = (-0.45, 0.5)$. Similar behavior occurs in region Ib, as shown in the figure for point B where $(h_R, h_I) = (-2.0, 1.5)$. Although the figure shows that the continuation of the two-point function away from integer values can be negative, note that the values at integer points are all non-negative. The two-point function at point C in region II where $(h_R, h_I) = (0.25, 1.25)$ shows the damped oscillatory behavior associated with $\mathcal{PT}$ breaking in excited states. For the point D in region III, where $(h_R, h_I) = (-0.5, 0.875)$, the $\mathcal{PT}$ breaking of the ground state leads to oscillatory behavior of the two-point function in the limit of large distance. Note that region III only occurs when $h_R$ is negative. For $h_R < 0$ and $h_I = 0$, the spin configurations with lowest energy have a two-fold degeneracy. With $h_I = 0$, the ground state of the transfer matrix is unique. For the case $h_R < 0$, $h_I = 0$, and $J$ large, the splitting of the two lowest eigenvalues of the transfer matrix in $d = 1$ is small. For sufficiently strong $h_I$, the real parts of the two lowest eigenvalues of $T$ merge, and $\mathcal{PT}$ symmetry breaking of the ground state occurs.

$\mathcal{PT}$ symmetry is not always manifest in the Hamiltonian or transfer matrix. A simple criterion for a $\mathcal{PT}$-symmetric Hamiltonian $H$ (or transfer matrix $T$) has been given by Bender and Mannheim [17]. If the characteristic polynomial $\det[H - \lambda I]$ has real coefficients, then $H$ has a generalized $\mathcal{PT}$ symmetry. In the case where $H$ is real, interesting models arise when $H$ is not symmetric. A notable example of this behavior is the ANNNI model [18]. The behavior seen above in the $d = 1$ $Z(3)$ model is quite general. There are generically three regions in $\mathcal{PT}$-symmetric models: region I, in which $\mathcal{PT}$ symmetry is unbroken;
region II, in which $\mathcal{PT}$ symmetry is broken by one or more pairs of excited states becoming complex; and region III, in which $\mathcal{PT}$ symmetry is broken by the ground state becoming complex. In region II, thermodynamic properties are unaffected, but oscillatory behaviors appears in correlation functions. In region III, the system is in a spatially modulated phase. We wish to emphasize that the behavior of correlation functions seen in regions II and III cannot be obtained from classical spin models for which $H$ is Hermitian: such behavior is incompatible with the spectral representation of the the correlation function for Hermitian theories.

IV. ZEROS OF THE PARTITION FUNCTION IN REGION 3

The change from region I to region II is generally not a phase transition in the thermodynamic limit. Within a transfer matrix framework, the largest eigenvalue is unique and real in both regions, so thermodynamic behavior is smooth. The change only appears in correlation functions. In condensed matter physics, the locus of points in parameter space where the change from region I to region II occurs has been known in statistical physics for
some time \cite{19} and is often called the disorder line. The transition from region I or II to
region III is generically a first-order phase transition. There is a general theory of parti-
tion function zeros that can be applied to $\mathcal{PT}$-symmetric lattice models \cite{20}. Under some
technical conditions, the partition function in a periodic volume $V = L^d$ can be written as

$$Z = \sum_m e^{-\beta V f_m} + \mathcal{O} \left( e^{-L/L_0} e^{-\beta V f} \right)$$

(8)

where $f = \min_m Re \left[ f_m \right]$ and $L_0$ is of the order of the largest correlation length of the system.
The $f_m$'s have the interpretation of complex free energy densities, and are independent of $L$.
These phases are stable if $Re \left(f_m\right) = f$ or metastable otherwise. The zeros of the partition
function are within $\mathcal{O} \left( e^{-L/L_0} \right)$ of the solutions of the equations.

$$Re \left(f_m\right) = Re \left(f_n\right) = f$$

$$Im \left(f_m\right) = Im \left(f_n\right) + (2p + 1) \frac{\pi}{\beta V}$$

for some $m \neq n$ and $p \in \mathbb{Z}$. We can apply this directly to region III, using the representation

$$Z = \sum_r e^{-LE_r} + \sum_p \left( e^{-LE_p} + e^{-LE_p^*} \right)$$

(9)

of the partition function. We identify $LE_0$ and $LE_0^*$ as $\beta L^d f_0$ and $\beta L^d f_0^*$, so that the
partition function has a zero for values of the parameters such that

$$\beta Im \left[f_0\right] = \frac{(2p + 1) \pi}{2V}$$

(10)

This tells us that the zeros of the partition function lie on the boundary of region III, defined
by $Im \left[f_0\right] = 0$, in the limit $V \to \infty$. As the volume of the system is taken to infinity, the
zeros of the partition function lie asymptotically on the boundary between phases. Note
that this analysis depends on $L_0$ remaining finite. At a 2nd-order transition, $L_0$ goes to
infinity and the approximation is invalid.

V. TOWARDS A SOLUTION OF THE SIGN PROBLEM

The difficulty presented by the sign problem depends directly on $\mathcal{PT}$ symmetry breaking
or its absence. Mostafazadeh has proven that when $\mathcal{PT}$ symmetry is unbroken (region I),
there is a similarity transformation $S$ that transforms a $\mathcal{PT}$-symmetric Hamiltonian $H$ into
an isospectral Hermitian Hamiltonian $H_h$ via $H_h = S H S^{-1}$ \cite{21}. This eliminates the sign
problem for $\mathcal{PT}$-symmetric quantum Hamiltonians throughout region I, if $S$ can be found. This theorem also applies to $\mathcal{PT}$-symmetric transfer matrices, but a further restriction to positive eigenvalues is necessary for the elimination of the sign problem.

In regions II and III, the sign problem has an underlying physical basis. The negative weight contributions to the partition function $Z$ arise from the contributions of complex conjugate eigenvalue pairs associated with $\mathcal{PT}$ symmetry breaking. It is that breaking that in turn gives rise to the oscillatory and damped oscillatory behavior of two-point functions characteristic of many physical systems. However, there are $\mathcal{PT}$ symmetric models like the ANNNI model [18] where the classical Hamiltonian, corresponding to the action in the path integral formalism, is real. Such a model can be simulated with no difficulties of principle throughout its parameter space. The key point is that the the transfer matrix is real but not symmetric. The existence of an antiunitary involution commuting with the Hamiltonian implies that there is a basis in which $H$ is real; see, e.g., [22]. This theorem easily extends to the case of those $\mathcal{PT}$-symmetric systems for which $\mathcal{PT}^2 = 1$, and can be applied to transfer matrices as well as Hamiltonians. This suggests the existence of a broad class of $\mathcal{PT}$-symmetric models which can be simulated in all three regions, but the extent of this class is as yet unknown.

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