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FISHER METRIC FOR DIAGONALIZABLE QUADRATIC HAMILTONIANS AND APPLICATION TO PHASE TRANSITIONS

TSVETAN VETSOV and RADOSLAV RASHKOV

Department of Physics, Kliment Ohridski University of Sofia, 1164 Sofia, Bulgaria

Abstract. We derive the extended entanglement entropy and the Fisher information metric in the case of quantum models, described by time-independent diagonal quadratic Hamiltonians. Our research is conducted within the framework of Thermo field dynamics. We also study the properties of the Fisher metric invariants to identify the phase structure of the quasi-particle systems in equilibrium.

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1. Introduction

One of the most challenging problems in modern physics is the intrinsic property of quantum systems to develop entanglement between their subsystems. A well-suited quantity, characterizing this process, is the geometric or entanglement entropy (EE), which is usually obtained by a trace over the degrees of freedom situated in a subspace of the whole system.

To better understand the intrinsic features of this kind of problems one can refer to the powerful tools of information geometry [1, 2]. The key concept here is the so-called Fisher information metric (FIM) [6], which defines a natural distance between different probability distributions, represented as points on a statistical manifold. By construction FIM can be defined as the Hessian of the entanglement entropy. Furthermore, the Fisher metric describes a continuous setting even if the underlying features of the system are discrete, which allows one to apply the classical methods of differential geometry as well.

Our interest is focused mainly on the study of quantum entanglement entropy and the Fisher information metric for generic bosonic systems in equilibrium, described by a diagonal time-independent quadratic Hamiltonians. The latter Hamiltonians often arise in important branches of physics such as condensed matter physics, quantum field theory and string theory.

Although one can always start with non-diagonal Hamiltonian, it is more efficient to work with diagonal matrices due to considerable simplification in the calculations of EE and FIM. For example, the Hamiltonian can be brought to diagonal form by an appropriate Bogoliubov transformation [4]. Such transformation mixes the creation and annihilation operators, but leaves the form of the commutation relations invariant. The new diagonal Hamiltonian now describes a quasi-particle system with a new set of creation and annihilation operators but the same energy eigenvalues as the original one.

In general it is difficult to calculate the entanglement entropy. However, the recent progress in Thermo field dynamics (TFD) [3, 13] offers relatively straightforward way of treating quantum states, which facilitates the derivation of the EE and the FIM. TFD requires the construction of a specific statistical state [7, 12]

$$|\Psi\rangle = \frac{1}{Z} \sum_{n} \mathrm{e}^{-\frac{\beta H}{2}} \, |n, \, \tilde{n}\rangle \tag{1}$$

defined in the so-called double Hilbert space, defined as a direct product of the original Hilbert space with basis $|n\rangle$ and an isomorphic copy of it with basis $|\tilde{n}\rangle$. Here $Z = Z(\beta)$ is the partition function and $\beta = 1/T$ is the inverse temperature. In [11] was shown that the extended state $|n, \, \tilde{n}\rangle \; = \; |n\rangle \bigotimes |\tilde{n}\rangle$ is invariant for any orthogonal complete set $\{|\alpha\rangle\}$, i.e., $\sum_n |n, \tilde{n}\rangle \; = \; \sum_\alpha |\alpha, \tilde{\alpha}\rangle$. Therefore the statistical state $|\Psi\rangle$ is independent of the chosen representation. This important result is known as “the general representation theorem” in TFD. It allows one to apply the TFD formalism even for non-equilibrium systems.

This paper is organized as follow. In Section 2 we calculate the extended entanglement entropy (EEE) and the Fisher information metric for bosonic systems in equilibrium, described by diagonal time-independent quadratic Hamiltonian. All calculations are conducted within the TFD formalism. In Section 3 we analyse the properties of the scalar curvature of the Fisher metric for two dimensional statistical manifold, spanned by the values of the inverse scaled temperatures. We apply that knowledge to identify the phase structure of the quasi-particle systems in equilibrium. We shortly summarize our results in Section 4.

2. Fisher Metric for Time-Independent Quadratic Hamiltonians

Let us consider bosonic quasi-particle systems whose phase structure can be explored by a two dimensional statistical manifold. In this case one can choose the following diagonal time-independent Hamiltonian

$$\widehat{H} = \sum_{n_{1,2}=0}^{\infty} (E_1\, n_1 + E_2\, n_2 + E_3\, n_3 + E_0)\, |n_1,\, n_2,\, n_3\rangle\, \langle n_1,\, n_2,\, n_3| \quad (2)$$

where E_0 is the energy in the ground state, while E_i, $i = 1, 2, 3$, are real energy coefficients, derived after some proper diagonalization procedure. The operator $\hat{n}_i = \hat{a}_i^\dagger\, \hat{a}_i$ is the i-th number operator built by the product of the creation and annihilation operators, satisfying standard commutation relations

$$[\hat{a}_i,\, \hat{a}_j^\dagger] = \delta_{ij}\,, \qquad [\hat{a}_i, \hat{a}_j] = [\hat{a}_i^\dagger, \hat{a}_j^\dagger] = 0, \qquad i,\, j = 1, 2, 3\,. \quad (3)$$

The Hilbert state vectors, $|\{n_i\}\rangle$, span the energy basis (the eigenvectors of the Hamiltonian)[1] with the following normalization condition

$$\langle m_1,\, m_2,\, m_3|n_1,\, n_2,\, n_3\rangle = \delta_{m_1,\, n_1}\, \delta_{m_2,\, n_2}\, \delta_{m_3,\, n_3}. \quad (4)$$

In order to find the entanglement entropy and the Fisher metric, we have to compute some relevant statistical quantities. The first such quantity is the partition function Z, which is straightforward to compute

$$\begin{aligned} Z(K_1,\, K_2) = \mathrm{Tr}_{1,2,3}\widehat{\mathrm{e}^{-\beta\, H}} &= \sum_{\ell_{1,2,3}=0}^{\infty} \langle \ell_1,\, \ell_2,\, \ell_3|\widehat{\mathrm{e}^{-\beta\, H}}\, |\ell_1,\, \ell_2,\, \ell_3\rangle \\ &= \frac{\mathrm{e}^{-K_0}}{(1-\mathrm{e}^{-K_1})\, (1-\mathrm{e}^{-K_2})\, (1-\mathrm{e}^{-K_3})} \end{aligned} \quad (5)$$

where $K_0 = \beta\, E_0$, $K_i = \beta\, E_i$, $i = 1, 2, 3$, are the so-called inverse scaled temperatures, and $\beta = 1/T$, ($k_B = 1$). The ordinary density matrix in equilibrium follows immediately

$$\widehat{\rho}_{eq}(K_1,\, K_2) = \frac{\widehat{\mathrm{e}^{-\beta\, H}}}{Z} = \frac{1}{Z} \sum_{n_{1,2,3}=0}^{\infty} \mathrm{e}^{-\sum\limits_{i=1}^{3} K_i\, n_i + K_0}\, |n_1,\, n_2,\, n_3\rangle\, \langle n_1,\, n_2,\, n_3|\,. \quad (6)$$

In the TFD formulation one introduces fictitious system, which is an isomorphic copy of the original quantum one, thus doubling the size of the Hilbert space. This

[1]The energy basis in this case is not essential, due to the general representation theorem in TFD.

trick leads to the definition of the following statistical state $|\Psi\rangle$

$$\begin{aligned} |\Psi\rangle &= \sum_{n_{1,2,3}=0}^{\infty} \sqrt{\rho_{eq}}\, |n_1,\, n_2,\, n_3\rangle\, |\tilde{n}_1,\, \tilde{n}_2,\, \tilde{n}_3\rangle \\ &= \frac{1}{\sqrt{Z}} \sum_{n_{1,2,3}=0}^{\infty} \mathrm{e}^{-\frac{1}{2}\,(K_1\, n_1 + K_2\, n_2 + K_3\, n_3 + K_0)}\, |n_1,\, n_2,\, n_3\rangle\, |\tilde{n}_1,\, \tilde{n}_2,\, \tilde{n}_3\rangle\, . \end{aligned} \tag{7}$$

One can now use (7) to compose the matrix elements of an extended density operator as follow

$$\begin{aligned} \widehat{\rho} = |\Psi\rangle\, \langle\Psi| = \frac{1}{Z} \sum_{n_{1,2,3}=0}^{\infty} \sum_{m_{1,2,3}=0}^{\infty} \mathrm{e}^{-\frac{1}{2}\,(K_1\,(n_1+m_1)+K_2\,(n_2+m_2)+K_3\,(n_3+m_3)+2\,K_0)} \\ \times |n_1,\, n_2,\, n_3\rangle\, \langle m_1,\, m_2,\, m_3|\, |\tilde{n}_1,\, \tilde{n}_2,\, \tilde{n}_3\rangle\, \langle \tilde{m}_1,\, \tilde{m}_2,\, \tilde{m}_3|\, . \end{aligned} \tag{8}$$

By assumption the system is in equilibrium, therefore of interest to us is only the quantum entanglement between its subsystems. Partitioning of quantum systems is not unique and depends on their intrinsic granularity. For our purpose one can choose a bipartite system, namely

$$\{n_1,\, n_2,\, n_3\} = \{n_1,\, n_2\} + \{n_3\} = A + B \tag{9}$$

traditionally called “Alice” and “Bob”. After this simple partitioning one can trace out the degrees of freedom in Bob’s subsystem, so that only the degrees of freedom seen by Alice remain

$$\begin{aligned} \widehat{\rho}_A = \mathrm{Tr}_{\mathrm{B}} \widehat{\rho} &= \sum_{\ell_3=0}^{\infty} \sum_{\tilde{\ell}_3=0}^{\infty} \langle \ell_3| \langle \tilde{\ell}_3 | \widehat{\rho} | \ell_3 \rangle\, |\tilde{\ell}_3\rangle \\ &= \left(\mathrm{e}^{K_1} - 1\right)\, \left(\mathrm{e}^{K_2} - 1\right) \sum_{n_{1,2}=0}^{\infty} \sum_{m_{1,2}=0}^{\infty} \mathrm{e}^{-\frac{K_1\,(2+n_1+m_1)+K_2\,(2+n_2+m_2)}{2}} \\ &\quad \times |n_1,\, n_2\rangle\, \langle m_1,\, m_2|\, |\tilde{n}_1,\, \tilde{n}_2\rangle\, \langle \tilde{m}_1,\, \tilde{m}_2|\, . \end{aligned} \tag{10}$$

Finally, tracing over the degrees of freedom in system A, one is left with the extended entanglement entropy between Alice’s and Bob’s subsystems

$$\begin{aligned} S_A\,(K_1,\, K_2) &= -\mathrm{Tr}_{\mathrm{A}}\,(\hat{\rho}_A \log \hat{\rho}_A) \\ &= \frac{1}{2} \coth\frac{K_1}{4} \coth\frac{K_2}{4} \left(K_1 \left(1 + \coth\frac{K_1}{4}\right) - 2 \ln\left(\mathrm{e}^{K_1} - 1\right)\right) \\ &\quad + \frac{1}{2} \coth\frac{K_1}{4} \coth\frac{K_2}{4} \left(K_2 \left(1 + \coth\frac{K_2}{4}\right) - 2 \ln\left(\mathrm{e}^{K_2} - 1\right)\right) . \end{aligned} \tag{11}$$

Equation (11) allows us to calculate the Fisher information metric. It can be expressed as the Hessian of the entanglement entropy [8,9]

$$g_{ab} = \frac{\partial^2 S_A}{\partial K_a \, \partial K_b}\,, \qquad a,\, b = 1, 2\,. \tag{12}$$

Explicitly one has the following expressions for the components of the metric

$$\begin{aligned} g_{11} &= \frac{1}{64}\,\coth\frac{K_2}{4}\,\mathrm{csch}^2\frac{K_1}{4}\left[K_1\left(3 + 5\coth^2\frac{K_1}{4} + 7\,\mathrm{csch}^2\frac{K_1}{4}\right)\right. \\ &\quad + 4\tanh\frac{K_1}{4} + 4\coth\frac{K_1}{4}\left(K_1 - 5 + K_2\left(1 + \coth\frac{K_2}{4}\right)\right. \\ &\quad \left.\left. - 2\log\left[\left(\mathrm{e}^{K_1} - 1\right)\left(\mathrm{e}^{K_2} - 1\right)\right]\right)\right] \end{aligned} \tag{13}$$

$$\begin{aligned} g_{12} = g_{21} &= \frac{1}{32}\,\mathrm{csch}^2\frac{K_1}{4}\,\mathrm{csch}^2\frac{K_2}{4}\left[K_1\left(1 + 2\coth\frac{K_1}{4}\right)\right. \\ &\quad \left. + K_2\left(1 + 2\coth\frac{K_2}{4}\right) - 2\log\left[\left(\mathrm{e}^{K_1} - 1\right)\left(\mathrm{e}^{K_2} - 1\right)\right] - 4\right] \end{aligned} \tag{14}$$

$$\begin{aligned} g_{22} &= \frac{1}{64}\,\coth\frac{K_1}{4}\,\mathrm{csch}^2\frac{K_2}{4}\left[K_2\left(3 + 5\coth^2\frac{K_2}{4} + 7\,\mathrm{csch}^2\frac{K_2}{4}\right)\right. \\ &\quad + 4\tanh\frac{K_2}{4} + 4\coth\frac{K_2}{4}\left(K_2 - 5 + K_1\left(1 + \coth\frac{K_1}{4}\right)\right. \\ &\quad \left.\left. - 2\log\left[\left(\mathrm{e}^{K_1} - 1\right)\left(\mathrm{e}^{K_2} - 1\right)\right]\right)\right]. \end{aligned} \tag{15}$$

The metric components are positive defined by construction, which is a necessary condition for thermodynamic stability (see [10] and references therein). From information-theoretic point of view the Fisher metric represents a continuous setting even if the underlying features of the system are discrete. This allows one to take advantage of the powerful framework of differential geometry to treat statistical structures as geometrical ones.

In our case the parameter space, spanned by the inverse scaled temperatures (K_1, K_2), is now two dimensional. Therefore one can study the parameter manifold by only investigating the properties of its scalar curvature. The latter is well known result in differential geometry, where in $2d$ space the Riemannian and Ricci curvatures are just multiples of the scalar curvature, e.g. there is only one degree of freedom. In the following section we investigate the properties of the Ricci invariant of the Fisher metric and comment on its relation to the strength of the interactions and the critical phase points in the quasi-system.

3. Applications to Phase Transitions

It is known fact that FIM defines a Riemannian metric on the space of parameters [1, 2, 6] for variety of statistical systems. Such geometrization is often useful in the analysis of the phase structure for number of statistical models [5, 10]. Here the scalar curvature, R, plays a crucial role, e.g. a non-interacting model shows flat geometry ($R = 0$), while the curvature diverges at the critical points of an interacting one.

An advantage of the probabilistic description of the system's phase structure is that it does not necessary require the existence of order parameters. This is useful for analysing systems, where such parameter is difficult to identify.

In this section we analyse the scalar curvature, $R = R_{ab}\, g^{ab}$, of the Fisher information metric (12), where $R_{ab} = R^{c}{}_{acb}$ is the Ricci tensor and

$$R_{abcd} = \frac{R}{2}\,(g_{ac}\, g_{bd} - g_{bc}\, g_{ad}) \tag{16}$$

is the Riemann curvature tensor in two dimensions. It is well-established that in two dimensions there is only one independent component of the curvature tensor, say R_{1212}, thus the Riemann tensor and the Ricci scalar are related by

$$R = \frac{2\, R_{1212}}{g_{11}\, g_{22} - g_{12}\, g_{21}}. \tag{17}$$

The explicit expression for R is too lengthy to be presented here. However its graphical representation near the origin ($K_1 = K_2 = 0$) is shown in Fig. 1.

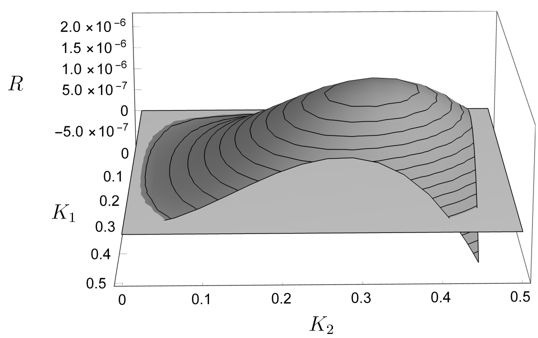

Figure 1. The Ricci scalar curvature R for high temperatures (low inverse scaled temperatures, $K_1, K_2 < 1$). The curvature is positive defined implying elliptic geometry on the statistical manifold. The local maximum of the curvature depicts the strongest interactions between the constituents of the quasi-system.

One notes that in this region the Ricci scalar is positive defined. The positive scalar curvature suggest elliptic geometry in the thermodynamic parameter space, while the local maximum corresponds to the strongest interaction between the constituents of the quasi-system.

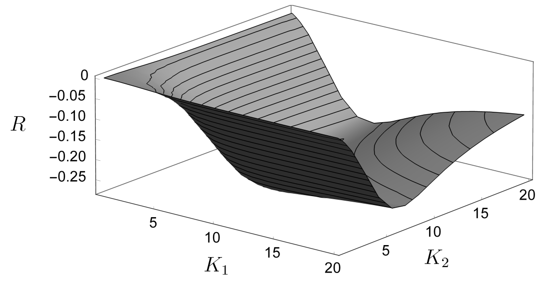

Figure 2. The Ricci scalar curvature R far from the origin, $K_1, K_2 > 1$. The curvature is negative implying hyperbolic geometry on the statistical manifold. The absolute value of the local minimum of the curvature depicts the strongest interactions between the constituents of the quasi-system.

For large values of the inverse scaled parameters (lower temperatures) the Ricci scalar is not positive defined as shown in Fig. 2.

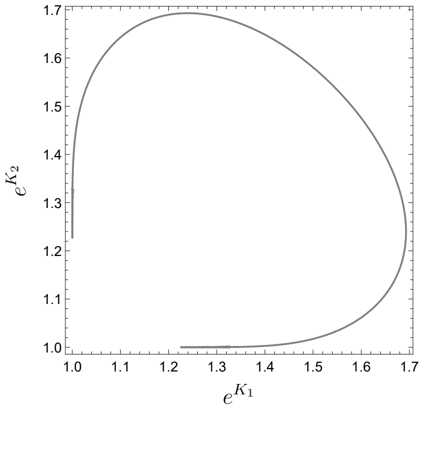

Figure 3. Free quasi-system, $R = 0$.

In this case the geometry in the space of parameters is hyperbolic. The absolute value of the local minimum of R corresponds to the strongest interactions in the hyperbolic case.

There is a level curve along which the scalar curvature is zero, thus separating the hyperbolic from the elliptic case as shown in Fig. 3.

The latter depicts flat geometry corresponding to free non-interacting quasi-system. There are also two more non-singular flat cases, namely at the origin and at infinity.

The smooth, non-singular behaviour of the $2d$ scalar curvature R, for all points on the parameter space (all physically admissible values of $K_{1,2}$), implies that the quasi-system, described by the Hamiltonian from equation (2), is thermodynamically stable and does not undergo any second order phase transitions. However, the Fisher metric is singular at the origin (for very high temperatures), which suggests that at this particular point the system may undergo a first order phase transition.

4. Conclusion

In this work we have found explicit expressions for the extended entanglement entropy and the Fisher information metric for quantum models, described by particular diagonal quadratic Hamiltonian. The investigation has been conducted for systems in thermal equilibrium and within the framework of Thermo field dynamics.

The analytical and the graphical study of the $2d$ information scalar curvature depicted three different geometric regions, corresponding to the type of the interactions between the constituents of the quasi-system.

Near the origin (for high temperatures) the scalar curvature is positive suggesting an elliptic type of geometry on the statistical manifold. The absolute value of the depicted local maximum corresponds to particular temperatures for which the interactions in the system are at their maximum strength.

Far from the origin (for lower temperatures) the geometry on the statistical manifold is hyperbolic (negative scalar curvature). The absolute value of the graphically depicted local minimum corresponds to the maximum strength of the interactions in the hyperbolic case.

The thin curvature line, separating the elliptic and the hyperbolic geometries, corresponds to flat statistical manifold. According to the established terminology this curve defines the temperatures at which the system is non-interacting. Flat geometry is found also at the origin point (infinite temperature) and at infinity (zero temperature).

The analysis also showed that the scalar curvature contains no singularities, thus effectively rendering the quasi-system thermodynamically stable. In other words, there are no critical phase points for which the system can undergo a second order phase transition. This result is necessary, but not sufficient to dismiss the existence of such points in the system. This is due to many factors, one of which is the choice of thermal parameters, in this case the inverse scaled temperatures, which may not be sensitive to some physically important features of the system. In this case a change of coordinates may be appropriate.

Finally, we consider the investigation of non-equilibrium systems with the methods presented in this paper, to be more important and interesting with wide scope of applications. We intend to conduct such investigation in the near future.

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