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Density functional fidelity susceptibility and Kullback–Leibler entropy

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ABSTRACT

It is shown that density functional fidelity susceptibility is approximately proportional to the relative or Kullback–Leibler entropy. A nearly linear relationship between the relative entropy and density functional fidelity is explored. The ratio of the fidelity and the distance of the relative entropy from 1 detects quantum phase transition. This is illustrated by numerical and analytical variational approximations for the ground state of the single-mode Dicke model.

Recently, quantum fidelity [1] has received a growing attention. This important concept of quantum information theory measures the similarity between two states. It has an important role in detecting quantum phase transitions (QPT) [2] as there is an abrupt change in the ground-state wave function at the transition point. (For a review of fidelity in QPT see [1].) Another important concept is the fidelity susceptibility [3]. It is the leading term of the fidelity.

For pure states fidelity is defined by the overlap between the states Ψ and Φ as

$$F(\Phi,\Psi)=\left|\langle\Phi|\Psi\rangle\right|. \tag{1}$$

Recently, there is an interest in connecting density functional theory and quantum phase transitions [4,5]. Analogously to Eq. (1), Gu [6] defined the density functional theory fidelity as the distance between two densities ϱ and σ:

$$f(\varrho,\sigma)=\int \varrho^{1/2}\sigma^{1/2}\,dq. \tag{2}$$

In this Letter continuous density distributions are considered. ϱ (or σ) is the density

$$\varrho(q)=\left|\Phi(q)\right|^2 \tag{3}$$

or in case of a many variable wave function

$$\varrho(q)=\int\left|\Phi(q,\tau)\right|^2 d\tau \tag{4}$$

is a reduced density. q and τ can denote several variables. For a many variable wave function, several reduced densities can be constructed. The following considerations are valid for any of them.

Quantum phase transition occurs when the ground-state energy and wave function undergo a significant change at a certain point. The ground-state wavefunction becomes qualitatively different across the transition point. Comparing the ground-state wavefunction or the density at two values of the control parameter (λ_1 and λ_2), "their distance" is large if λ_1 and λ_2 are on different sides of the transition point, and small if λ_1 and λ_2 are in the same phase. Consequently, fidelity shows a minimum at the transition point. Therefore, fidelity is generally considered at two close points λ and $\lambda+\delta\lambda$. An expansion around λ leads to the definition of fidelity susceptibility χ_F [6]

$$F(\lambda,\lambda+\delta\lambda)=1-\frac{1}{2}(\delta\lambda)^2\chi_F+\cdots. \tag{5}$$

Analogously, the dft fidelity susceptibility χ_f can be defined as the leading term of the dft fidelity:

$$f(\lambda,\lambda+\delta\lambda)=1-\frac{1}{2}(\delta\lambda)^2\chi_f+\cdots. \tag{6}$$

Expanding $\varrho(\lambda+\delta\lambda)$ around $\varrho(\lambda)$ we arrive at

$$\chi_f=\frac{1}{4}\int\frac{1}{\varrho}\left(\frac{\partial\varrho}{\partial\lambda}\right)^2 d\tau. \tag{7}$$

That is, the dft fidelity susceptibility is proportional to the Fisher information

$$I=\int\frac{1}{\varrho}\left(\frac{\partial\varrho}{\partial\lambda}\right)^2 d\tau. \tag{8}$$

The Fisher informational functional [7] is defined as a measure of the ability to estimate a parameter

$$I(\lambda)=\int p(x|\lambda)\left[\frac{\partial\ln p(x|\lambda)}{\partial\lambda}\right]^2 dx=\int\frac{[p'(x|\lambda)]^2}{p(x|\lambda)}\,dx. \tag{9}$$

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$p(x|\lambda)$ is a probability density function depending on a parameter λ. If λ is a parameter of locality

$$p(x|\lambda) = p(x+\lambda) = p(\gamma) \tag{10}$$

where $\gamma \equiv x+\lambda$ is a new variable. Therefore

$$\frac{\partial p(x|\lambda)}{\partial \lambda} = \frac{\partial p(x+\lambda)}{\partial (x+\lambda)} = \frac{\partial p(\gamma)}{\partial \gamma}. \tag{11}$$

As the expression does not depend on λ, we may set the locality at zero and the Fisher information takes the form:

$$I(\lambda=0) = \int \frac{[p'(x)]^2}{p(x)} dx. \tag{12}$$

Frequently, Eq. (12) is applied for Fisher information. However, if Eq. (10) is not valid, Eq. (9) should be applied. Selecting ϱ as a probability density function, we can immediately see that the density does not fulfil Eq. (10) and Eq. (8) gives the correct way of obtaining Fisher information.

Following the derivation of Frieden [8] we can find a link between fidelity susceptibility and the relative or Kullback–Leibler entropy [9]. The relative entropy is defined

$$I_{KL}(f,g) = \int f \ln \frac{f}{g} d\tau \tag{13}$$

for distribution functions f and g. This quantity measures the "distance" of the two distribution functions.

The Fisher information (8) can be rewritten as

$$\begin{aligned} I &= \lim_{\delta\lambda\to 0} \int \frac{1}{\varrho(\lambda)} \left(\frac{\varrho(\lambda+\delta\lambda) - \varrho(\lambda)}{\delta\lambda} \right)^2 d\tau \\ &= \lim_{\delta\lambda\to 0} \frac{1}{(\delta\lambda)^2} \int \varrho(\lambda) \left[\frac{\varrho(\lambda+\delta\lambda)}{\varrho(\lambda)} - 1 \right]^2 d\tau. \end{aligned} \tag{14}$$

Introducing the small quantity $\nu = \varrho(\lambda+\delta\lambda)/\varrho(\lambda) - 1$ and using the expansion $\ln(1+\nu) = \nu - \nu^2/2$, we arrive at

$$I \approx -\frac{2}{(\delta\lambda)^2} \int \varrho(\lambda) \ln \frac{\varrho(\lambda+\delta\lambda)}{\varrho(\lambda)} d\tau. \tag{15}$$

Therefore, dft fidelity susceptibility can be rewritten as

$$\chi = -\frac{2}{(\delta\lambda)^2} \int \varrho(\lambda) \ln \frac{\varrho(\lambda+\delta\lambda)}{\varrho(\lambda)} d\tau, \tag{16}$$

or

$$\chi = \frac{2}{(\delta\lambda)^2} I_{KL}\big(\varrho(\lambda), \varrho(\lambda+\delta\lambda)\big). \tag{17}$$

That is, dft fidelity susceptibility is proportional to the relative or Kullback–Leibler entropy. From the definition (6) follows the linear relationship between the relative entropy and dft fidelity

$$I_{KL}\big(\varrho(\lambda), \varrho(\lambda+\delta\lambda)\big) = 1 - f(\lambda, \lambda+\delta\lambda). \tag{18}$$

In a QPT the wavefunction has an abrupt change in the critical point and the approximation (15) will be worse in this point. Nevertheless, we can use the Kullback–Leibler entropy instead of the fidelity as a detector of a quantum phase transition. We define a new quantity

$$C(\lambda, \delta\lambda) \equiv f(\lambda, \lambda+\delta\lambda) / \big(1 - I_{KL}\big(\varrho(\lambda), \varrho(\lambda+\delta\lambda)\big)\big) \tag{19}$$

measuring the quality of the relation (18). $C(\lambda, \delta\lambda)$ is approximately 1 except around a region at the critical point, where it will move away from 1. To illustrate these properties the single-mode Dicke model in considered. We mention in passing that entropic quantities have recently been found good markers of QPT [10–16].

The Dicke model [17–20] describes an ensemble of N two-level atoms, with level splitting ω_0, interacting with an electromagnetic field with frequency ω. The Hamiltonian is given by

$$H = \omega_0 J_z + \omega a^\dagger a + \frac{\lambda}{\sqrt{2j}} \big(a^\dagger + a\big)(J_+ + J_-), \tag{20}$$

where J_z, $J_\pm$ are the angular momentum operators for a pseudospin of length $j = N/2$, and a and $a^\dagger$ are the bosonic operators of the field, and λ is the coupling parameter for the dipolar interaction between the field and the atoms. It is known that there is a quantum phase transition for $\lambda = \lambda_c = \frac{\sqrt{\omega\omega_0}}{2}$ in the thermodynamic limit ($N \to \infty$, with two phases, the normal phase ($\lambda < \lambda_c$) and the superradiant phase ($\lambda > \lambda_c$)). The parity operator $\hat{\Pi} = e^{i\pi(a^\dagger a + J_z + j)}$ commutes with H and, in particular, the ground state must be an even parity one.

We solve the problem numerically (diagonalizing the Hamiltonian) and analytically (with a variational approximation). For this purpose a basis set $\{|n; j, m\rangle \equiv |n\rangle \otimes |j, m\rangle\}$ of the Hilbert space is introduced, with $\{|n\rangle\}_{n=0}^{\infty}$ the number states of the field and $\{|j, m\rangle\}_{m=-j}^{j}$ the so-called Dicke states of the atomic sector. Any vector ψ can be expanded in terms of the basis as

$$|\psi\rangle = \sum_{n=0}^{n_c} \sum_{m=-j}^{j} c_{nm}^{(j)} |n; j, m\rangle \tag{21}$$

where the coefficients $c_{nm}^{(j)}$ are calculated by numerical diagonalization and the bosonic Hilbert space is truncated with a given cutoff n_c (which is chosen by minimizing the energy).

With the Holstein–Primakoff approximation (see [21]), the wavefunction in position representation is

$$\begin{aligned} \psi(x, y) &= \sqrt{\omega\omega_0} e^{-\frac{1}{2}(\omega x^2 + \omega_0 y^2)} \sum_{n=0}^{n_c} \sum_{m=-j}^{j} c_{nm}^{(j)} \\ &\quad \times \frac{H_n(\sqrt{\omega}x) H_{j+m}(\sqrt{\omega_0}y)}{2^{(n+m+j)/2} \sqrt{n!(j+m)!}}, \end{aligned} \tag{22}$$

where we have used the representation of the field and atomic sectors:

$$\begin{aligned} \langle x|n\rangle &= \sqrt{\omega} e^{-\frac{1}{2}\omega x^2} \frac{H_n(\sqrt{\omega}x)}{\sqrt{2^n n! \sqrt{\pi}}}, \\ \langle y|j, m\rangle &= \sqrt{\omega_0} e^{-\frac{1}{2}\omega_0 y^2} \frac{H_{j+m}(\sqrt{\omega_0}y)}{\sqrt{2^{(j+m)}(j+m)! \sqrt{\pi}}}. \end{aligned} \tag{23}$$

Additionally, an analytical variational approximation for the ground state of the Dicke model, is expressed in terms of the parity symmetry adapted coherent states introduced by Castaños et al. [22,23]

$$|\psi_v\rangle = \frac{|\alpha\rangle \otimes |z\rangle + |-\alpha\rangle \otimes |-z\rangle}{\mathcal{N}(\alpha, z)}, \tag{24}$$

where $|\alpha\rangle \otimes |z\rangle$ (with $\alpha, z \in \mathbb{C}$) are the standard (canonical or Glauber) and spin-j Coherent States (CSs) for the photon and the particle sectors given by [22,23]

$$\begin{aligned} |\alpha\rangle &= e^{-|\alpha|^2/2} e^{\alpha a^\dagger} |0\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle, \\ |z\rangle &= \big(1 + |z|^2\big)^{-j} e^{z J_+} |j, -j\rangle \\ &= \big(1 + |z|^2\big)^{-j} \sum_{m=-j}^{j} \binom{2j}{j+m}^{1/2} z^{j+m} |j, m\rangle, \end{aligned} \tag{25}$$