Quantum phase transitions via density functional theory. Extension to degenerate case

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According to the recently proposed density functional analogue of the quantum phase transitions the 'density' determines the 'control parameter' (corresponding to the Density Functional Theory 'external potential'). It is also proved that in the non-degenerate case there is a one-to-one map between the ground-state wave function and the control parameter. It is now shown that there is a one-to-one map between the ground-state subspace and the control parameter. It is pointed out that there is a one-to one map between the 'subspace density' and the 'control parameter'. The Rényi entropies are proved to be strictly monotonous functions of the control parameter in a neighborhood of the transition point. These properties are illustrated with the Dicke model which exhibits a QPT from a normal phase (non-degenerate) to a superradiant case (degenerate) in the thermodynamic limit.

keywords: quantum phase transitions, density functional theory, subspace density, Rényi entropy, Dicke model

Quantum phase transitions (QPT) are extensions of classical phase transitions to zero absolute temperature. Quantum fluctuations, induced by a variation in the values of certain control parameter(s), lead to an abrupt change in the physical properties of the system [1]. On the other hand, density functional theory (DFT) (initiated by Hohenberg and Kohn [2–4]) provides the density as the basic variable to obtain properties of many particle systems. So the DFT can be used to study QPT. In fact, DFT has been shown to provide a relationship between QPT and entanglement and it has been introduced an analogue of the DFT density and showed that this new 'density' determines the control parameter(s) in QPTs [8]. Entanglement has also been studied in the density functional theory [5–7].

Recently, following the idea of Wu et al. [8], a DFT visualization of QPTs has been extended [9] with the constraint search approach. It has been proved that, in non-degenerate ground state, there is a bijective map between the density function and the control parameter(s). Moreover, any strictly monotonous functional provides us a new 'density' with a different control parameter (or DFT 'external potential'), which is determined by the new 'density'. In particular, a bijection between the Rényi entropy and the control parameter has been considered. In this paper we will generalize all these results for a degenerate ground state subspace.

Consider the Hamiltonian

$$\hat{H} = \hat{T} + \hat{V}_{ee} + \sum_{i=1}^{N} v(\mathbf{r}_i) \,, \tag{1}$$

where $\hat{T}$ and $\hat{V}_{ee}$ are the kinetic energy and the electron-electron energy operators, respectively. The Schrödinger equation can be written as

$$\hat{H}|\Psi_\gamma\rangle = E|\Psi_\gamma\rangle \qquad (\gamma = 1, 2, \ldots, g) \,, \tag{2}$$

where g is the degeneracy. The wave functions Ψ_γ span the subspace S of the Hilbert space. Instead of the wave functions Ψ_γ any other set of wave functions obtained from a unitary transformation can be used. The total energy can be considered as a functional of the subspace S. We can also construct density matrices in the subspace S [10–13]:

$$\hat{D} = \sum_{\gamma=1}^{g} w_\gamma |\Psi_\gamma\rangle\langle\Psi_\gamma| \,. \tag{3}$$

The weighting factors w_γ should satisfy the conditions

$$1 = \sum_{\gamma=1}^{g} w_\gamma \tag{4}$$

and

$$w_\gamma \geq 0 \,. \tag{5}$$

The subspace (ensemble) density is given by

$$\varrho = \sum_{\gamma=1}^{g} w_\gamma \int |\Psi_\gamma|^2 ds_1 d\mathbf{x_2} ... d\mathbf{x_N} \,, \tag{6}$$

where $\mathbf{x}$ stands for both the coordinates and the spin. Selecting the weighting factors to be equal, the subspace density has the symmetry of the external potential.

The energy can be written as

$$E = F + \int \varrho(\mathbf{r}) v(\mathbf{r}) d\mathbf{r}, \tag{7}$$

where the functional F is the sum of the kinetic and electron-electron repulsion energies. The ground-state energy is then obtained by minimizing the energy in Eq.

(7). The constrained-search formalism [14, 15] can be used as follows:

$$E[\varrho] = \min_{S} \sum_{\gamma=1}^{g} w_\gamma \langle \Psi_\gamma | \hat{H} | \Psi_\gamma \rangle$$
$$= \min_{\varrho} \left\{ \min_{S\to\varrho} \sum_{\gamma=1}^{g} w_\gamma \langle \Psi_\gamma | \hat{H} | \Psi_\gamma \rangle \right\}$$
$$= \min_{\varrho} \left\{ F[\varrho] + \int \varrho(\mathbf{r}) v(\mathbf{r}) d\mathbf{r} \right\} . \quad (8)$$

The functional $F[\varrho]$ can be expressed with the density matrix as

$$F[\varrho] = \min_{S\to\varrho} tr \left\{ \hat{D}(\hat{T} + \hat{V}_{ee}) \right\} . \quad (9)$$

Then the generalized Hohenberg-Kohn theorem has the form

$$F[\varrho] + \int \varrho(\mathbf{r}) v(\mathbf{r}) d\mathbf{r} \geq E_0, \quad (10)$$

that can be readily proved as follows:

$$F[\varrho] + \int \varrho(\mathbf{r}) v(\mathbf{r}) d\mathbf{r} = \min_{S\to\varrho} tr \left\{ \hat{D}(\hat{T} + \hat{V}_{ee}) \right\} +$$
$$\int \varrho(\mathbf{r}) v(\mathbf{r}) d\mathbf{r} = \min_{S\to\varrho} tr \left\{ \hat{D}(\hat{T} + \hat{V} + \hat{V}_{ee}) \right\} \geq E_0, \quad (11)$$

where the last inequality follows from the variational principle. There is an equality if and only if the trial subspace density ϱ is equal to the true subspace density. The functional derivative of F gives the external potential up to a constant

$$\frac{\delta F[\varrho]}{\delta \varrho} = -v(\mathbf{r}). \quad (12)$$

We would like to emphasize that it is crucial to use subspace densities to ensure the one-to-one map between the density and the potential. If we use the degenerate densities (corresponding to the degenerate wave functions) instead of the subspace density, a given density does generally not correspond to a unique ground state and the map between the density and the potential is not invertible as the wave function is not unique functional of the density. Consequently the problem is subtler (see e.g.[16–18]. If, however, we use subspace densities, the problem is as simple as the nondegenerate problem.

Consider now a quantum system with the Hamiltonian

$$\hat{H} = \hat{H}_0 + \sum_i \xi_i \hat{A}_i, \quad (13)$$

where $\hat{H}_0$ is integrable and ξ_i are the control parameters associated with $\hat{A}_i$ [8, 19]. Note that $\hat{H}_0$ and $\hat{A}_i$ are known Hermitian operators. The index i is discrete. For a continuous case, the original DFT described above should be applied. We mention in passing that the idea of adding various operators to the Hamiltonian in a general density functional context was first discussed by Bauer [20]. The expectation value of $\hat{A}_i$ is given by

$$a_i = tr \left\{ \hat{D} \hat{A}_i \right\} . \quad (14)$$

The constrained search leads to the function

$$Q(\{a_i\}) = \underset{S\to\{a_i\}}{\mathrm{Min}} tr \left\{ \hat{D}\hat{H}_0 \right\} = \underset{\hat{D}\to\{a_i\}}{\mathrm{Min}} tr \left\{ \hat{D}\hat{H}_0 \right\} , \quad (15)$$

that is, the expectation value of the Hamiltonian $\hat{H}_0$ is minimized subject to the constraint that each D (or S) yields the given values a_i. Note that a_i are defined by the subspace of degenerate eigenfunctions, these corresponds to the 'subspace densities' of the original density functional theory, while ξ_i corresponds to the external potential.

The minimum of the energy is searched in two steps:

$$E = \underset{\{a_i\}}{\mathrm{Min}} \left[\underset{S\to\{a_i\}}{\mathrm{Min}} tr \left\{ \hat{D}\hat{H} \right\} \right]$$
$$= \underset{\{a_i\}}{\mathrm{Min}} \left[\underset{S\to\{a_i\}}{\mathrm{Min}} tr \left\{ \hat{D}\hat{H}_0 \right\} + \sum_i \xi_i a_i \right]$$
$$= \underset{\{a_i\}}{\mathrm{Min}} \left[Q(a_1, ..., a_M) + \sum_i \xi_i a_i \right] . \quad (16)$$

We can also see that Q is the Legendre transform of E:

$$Q(a_1, ..., a_M) = E - \sum_i \xi_i a_i. \quad (17)$$

From the Hellmann-Feynman theorem

$$\frac{\partial E}{\partial \xi_i} = tr \left\{ \hat{D} \frac{\partial \hat{H}}{\partial \xi_i} \right\} = tr \left\{ \hat{D} \hat{A}_i \right\} = a_i \quad (18)$$

follows that

$$\frac{\partial Q}{\partial a_i} = -\xi_i. \quad (19)$$

Theorem 1. *If the inverse of the operator* $\hat{P} = \sum_i c_i \hat{A}_i - c_0$ *exits for any real* c_0 *and* c_i*, there is a one-to-one map between the subspace* S *spanned by the degenerate wave functions* $\Psi_\gamma (\gamma = 1, 2, \ldots, g)$ *and the 'external potential'* $\{\xi_i\}$.

Proof: First, we prove that the 'external potential' $\{\xi_i\}$ determines the subspace S. If $\{\xi_i\}$ are known, the solution of the Schrödinger equation with the Hamiltonian (13) gives the wave functions Ψ_γ.

Second, we have to prove that the subspace S determines the 'external potential' $\{\xi_i\}$, that is, only one 'external potential' $\{\xi_i\}$ corresponds to a given S. The proof proceeds by reductio ad absurdum. Suppose that there are two 'external potentials' $\{\xi_i^{(1)}\}$ and $\{\xi_i^{(2)}\}$ with the

same subspace. The corresponding Schrödinger equations have the form

$$\hat{H}_{\xi^{(1)}}\Psi_\gamma = \left[\hat{H}_0 + \sum_i \xi_i^{(1)}\hat{A}_i\right]\Psi_\gamma = E^{(1)}\Psi_\gamma \tag{20}$$

and

$$\hat{H}_{\xi^{(2)}}\Psi'_\gamma = \left[\hat{H}_0 + \sum_i \xi_i^{(2)}\hat{A}_i\right]\Psi'_\gamma = E^{(2)}\Psi'_\gamma, \tag{21}$$

where $E^{(1)}$ and $E^{(2)}$ are the eigenvalues of the Hamiltonians $\hat{H}_0 + \sum_i \xi_i^{(1)}\hat{A}_i$ and $\hat{H}_0 + \sum_i \xi_i^{(2)}\hat{A}_i$, respectively. The wave functions Ψ_γ and wave functions Ψ'_γ with $\gamma = 1, 2, \ldots, g$ are related by a unitary transformation:

$$\Psi_\gamma = \sum_\kappa c_{\gamma\kappa}\Psi'_\kappa. \tag{22}$$

From Eqs. (20) and (22) we arrive at

$$\hat{H}_{\xi^{(1)}}\Psi_\gamma = \hat{H}_{\xi^{(1)}}\sum_\kappa c_{\gamma\kappa}\Psi'_\kappa = E^{(1)}\Psi_\gamma = E^{(1)}\sum_\kappa c_{\gamma\kappa}\Psi'_\kappa. \tag{23}$$

Combining Eqs. (20), (21) and (23) we are led to the equations

$$\hat{R}\sum_\kappa c_{\gamma\kappa}\Psi'_\kappa = (E^{(1)} - E^{(2)})\sum_\kappa c_{\gamma\kappa}\Psi'_\kappa, \tag{24}$$

where

$$\hat{R} = \sum_i (\xi_i^{(1)} - \xi_i^{(2)})\hat{A}_i. \tag{25}$$

The operator $\hat{R}$ maps the states of S into the states of S, that is, S is an invariant space of the operator $\hat{R}$. A theorem of the linear algebra states that if a Hermitian operator leaves a finite dimensional subspace invariant then this operator has eigenstates in this subspace [21]. But $\hat{R}$ has no eigenstates in the Hilbert space unless it is constant. We can immediately see it as follows: suppose that Φ is an eigenfunction of $\hat{R}$

$$\hat{R}\Phi = \lambda\Phi \tag{26}$$

or

$$\hat{G}\Phi = 0, \tag{27}$$

where

$$\hat{G} = \sum_i (\xi_i^{(1)} - \xi_i^{(2)})\hat{A}_i - \lambda. \tag{28}$$

We can exclude the solution of $\Phi = 0$ (everywhere or in a domain of nonzero measure). Eq. (27) gives the kernel $\hat{G}$. (The definition is $Ker\hat{G} = \{\Phi \in \mathcal{H} : \hat{G}\Phi = 0\}$, where $\mathcal{H}$ denotes the Hilbert space.) As the inverse of an operator $\hat{P} = \sum_i c_i\hat{A}_i - c_0$ exits for any real c_0 and c_i,the inverse of $\hat{G}$ also exits ($c_i = \xi_i^{(1)} - \xi_i^{(2)}$ and $c_0 = \lambda$). Therefore $Ker\hat{G} = \{0\}$ and it leads to $\xi_i^{(1)} = \xi_i^{(2)}$.□

The Hamiltonian (13) can be rewritten as

$$\hat{H} = \hat{H}_0 + \sum_i \zeta_i\hat{B}_i, \tag{29}$$

where $\hat{B}_i = \hat{A}_i\xi_i/\zeta_i$, $b_i = tr\left\{\hat{D}\hat{B}_i\right\} = a_i\xi_i/\zeta_i$ and $\zeta_i \neq 0$. We can reformulate theorem 1 as:

Corolary 1. *If $\zeta_i = f_i(\xi_i)$ and f_i are strictly monotonous functions, there is a one-to-one map between the subspace S and the 'external potential' $\{\zeta_i\}$.*

ζ_i are the 'new' control parameters associated with the 'new subspace density' b_i.

Theorem 2. *There is a one-to one map between the subspace spanned by 'subspace densities' $\{a_i\}$ and the 'external potential' $\{\xi_i\}$.*

Proof: If $\{\xi_i\}$ are known, the subspace density $\{a_i\}$ can be calculated from the Schrödinger equation with the Hamiltonian (13) and Eq. (14). If, on the other hand, the subspace density $\{a_i\}$ is available the subspace S should be first found by minimizing the expectation value of the Hamiltonian (see Eq. (15)). In the knowledge of S, we have to find $\{\xi_i\}$ for which any independent set of basis functions of S fulfills the Schrödinger equation. □

From Corollary 1 and Theorem 2 follows

Corolary 2. *If $\zeta_i = f_i(\xi_i)$ and f_i are strictly monotonous functions, there is a one-to-one map between the 'subspace density' b_i and the 'external potential' $\{\zeta_i\}$.*

Theorem 3.

$$Q(a_1, ..., a_M) + \sum_i \xi_i a_i \geq E_{gs}, \tag{30}$$

where E_{gs} is the ground-state energy of the Hamiltonian (13). Equality holds if and only if $\{a_i\}$ is the ground-state 'subspace density'.

Proof: See the constrained search approach [Eqs. (15) - (16)].

Corolary 3.

$$Q(b_1, ..., b_M) + \sum_i \zeta_i b_i \geq E_{gs}. \tag{31}$$

Equality holds iff $\{b_i\}$ is the 'new ground-state subspace density'.

The Rényi entropy is defined as

$$R^\alpha = \frac{1}{1-\alpha}\ln\int \rho^\alpha(q)dq \tag{32}$$

where $\alpha > 0$ and ρ is the normalized density. In the following the position representation of the wave function is utilized.

The ground state subspace density can be defined as

$$\rho(x) = \sum_{\gamma=1}^{g} w_\gamma |\Psi_\gamma(x)|^2 \tag{33}$$

or

$$\rho(x) = \sum_{\gamma=1}^{g} w_\gamma \int |\Psi_\gamma(x,q)|^2 dq, \tag{34}$$

that is, in case of a many variable wave function the Rényi entropy (32) can be determined for several (reduced) densities depending on how many variables (if any (33)) are integrated out (34). The following theorem is valid for any case.

As it was pointed out by Wu et al. [8] one can split Hamiltonian (13) in several ways. It is possible to focus on only one contol parameter and merge the other parts of the sum $\sum_i \xi_i \hat{A}_i$ into $\hat{H}_0$. Theorem 4 and corolary 4 is valid for this special case.

Theorem 4. *The Rényi entropy R^α of the ground state subspace density, if it exists, is a strictly monotonous (increasing or decreasing) function of the control parameter ξ in a neighborhood of the transition point ξ_c,and its derivative $dR^\alpha/d\xi$ diverges at ξ_c in the thermodynamic limit.*

Proof:

The Hamiltonian can be reformulated as $\mu = \xi - \xi_c$:

$$\hat{H} = \tilde{\hat{H}}_0 + \mu \hat{H}', \tag{35}$$

where $\tilde{\hat{H}}_0 = \hat{H}_0 + \xi_c \hat{A}$, $\hat{H}' = \hat{A}$ and $\mu = \xi - \xi_c$. It is enough to show that $\omega_\alpha \equiv \int \rho^\alpha(x) dx$ is a strictly monotonous function of μ in a neighborhood of $\mu = 0$. As the logarithm is an increasing function the Rényi entropy has the same monotonic behavior. In the perturbation theory the ground state wave function can be written as:

$$\Psi_\gamma = \Psi_\gamma^{(0)} + \mu \Psi_\gamma^{(1)} + O(\mu^2), \tag{36}$$

where the zero-order ($\Psi_\gamma^{(0)}$) and first-order ($\Psi_\gamma^{(1)}$) wave functions can be expressed with the degenerate non-perturbative eigenfunctions and eigenenergies.

Substituting Eq. (36) into Eqs (33) and (34) we arrive at

$$\rho = \rho_0 + \mu \rho_1 + O(\mu^2), \tag{37}$$

where

$$\rho_0 = \sum_{\gamma=1}^{g} w_\gamma |\Psi_\gamma^{(0)}|^2 \tag{38}$$

$$\rho_1 = 2 \sum_{\gamma=1}^{g} w_\gamma \mathrm{Re}[\Psi_\gamma^{(0)*} \Psi_\gamma^{(1)}] \tag{39}$$

in case 1 (Eq. (33)) and

$$\rho_0 = \sum_{\gamma=1}^{g} w_\gamma \int dq |\Psi_\gamma^{(0)}|^2 \tag{40}$$

$$\rho_1 = 2 \sum_{\gamma=1}^{g} w_\gamma \int dq \mathrm{Re}[\Psi_\gamma^{(0)*} \Psi_\gamma^{(1)}] \tag{41}$$

in case 2 (Eq. (34)). (Note that position representation is applied.) Finally, $\omega_\alpha(\mu)$ is expanded around $\mu = 0$

$$\omega_\alpha(\mu) = \omega_\alpha^{(0)} + \mu \alpha P + O(\mu^2) \tag{42}$$

with

$$\omega_\alpha^{(0)} = \int \rho_0^\alpha \tag{43}$$

and

$$P = \int \rho_0^{\alpha-1} \rho_1. \tag{44}$$

$\omega_\alpha^{(0)}$ and P are independent of μ. Thus, we have that $d\omega_\alpha/d\mu = \alpha P$. As P is non-zero (either strictly positive or negative) and, therefore, $\omega_\alpha(\mu)$ is strictly monotonous in a neighborhood of $\mu = 0$. It is shown in the Appendix that, in the thermodynamic limit (that is, when $E_k^{(0)} \to E_0^{(0)}$ for one or several values of k), P and consequently the functional derivative of the Rényi entropy diverge. □

Corolary 4. *As the Rényi entropy R^α is strictly monotonous function of ξ in the vicinity of the transition point, there is also a one-to-one map between the Rényi entropy of a given order R^α and the 'external potential' ξ.*

As an illustration of these results we will consider the Dicke model [22–25]. This model describes an ensemble of N two-level atoms with level splitting ω_0 coupled by a single-mode bosonic field with frequency ω and its hamiltonian has the form:

$$H = \omega_0 J_z + \omega a^\dagger a + \frac{\lambda}{\sqrt{2j}}(a^\dagger + a)(J_+ + J_-) \tag{45}$$

where J_z and $J_\pm$ are the angular momentum operators for a pseudospin of length $j = N/2$ and a and $a^\dagger$ are the photon annihilation and creation operators of the field. It is known that the Dicke model exhibits a second-order phase transition at the critical point $\lambda_c = \sqrt{\omega\omega_c}/2$ in the superradiant one in the thermodynamic limit $N \to \infty$, where the energy levels are nondegenerate in the normal phase and degenerate in the superradiant one [26].

Let us rewritten the Dicke model hamiltonian as

$$\hat{H} = \hat{H}_0 + \lambda \hat{A} \tag{46}$$

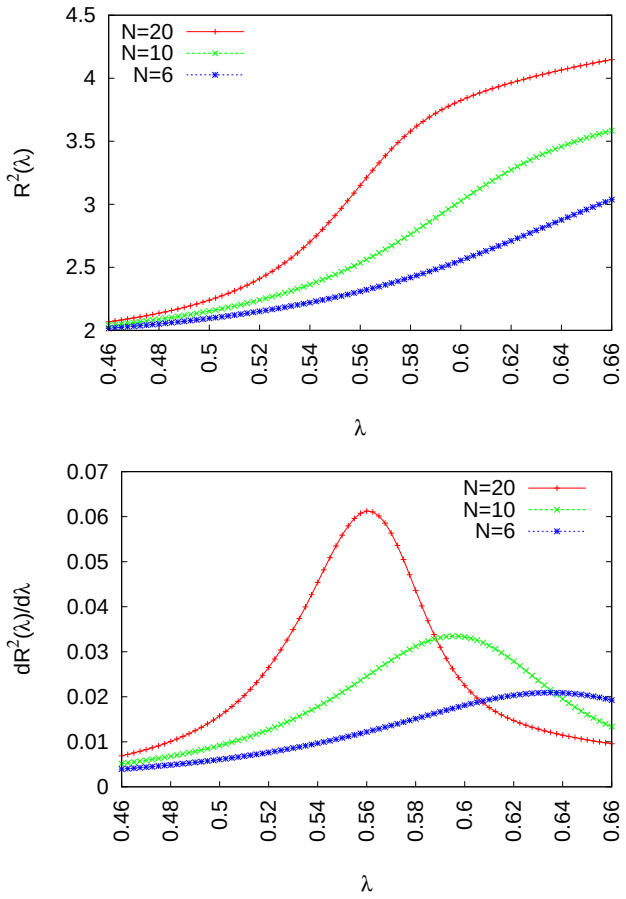

FIG. 1. (Color online) Rényi entropy $R^2(\lambda)$ (top) and derivative of the Rényi entropy $\frac{dR^2(\lambda)}{d\lambda}$ (bottom) as a function of the parameter λ for different values of $N = 6, 10$, and 20 for the Dicke Model and for $\omega_0 = \omega = 1$. (Atomic units).

where

$$\hat{H}_0 = \omega_0 J_z + \omega a^\dagger a, \qquad \hat{A} = \frac{1}{\sqrt{2j}}(a^\dagger + a)(J_+ + J_-). \quad (47)$$

Now, we can solve numerically the eigenvalue problem diagonalizing the matrix representation of the $\hat{H}$ operator (in the basis set of the Hilbert space $\{|n\rangle \otimes |jm\rangle\}$, with $\{|n\rangle\}_{n=0}^{\infty}$ the number states of the field and $\{|jm\rangle\}_{m=-j}^{j}$ the so-called Dicke states). See [27, 28] for more details and [29–33] for a study of the QPT in this model in terms of information measures.

In Fig. 1 we can see Rényi entropy R^2 of the ground state subspace density in the Dicke model as a function of the parameter λ around the transition point λ_c for different values of $N = 6$, 10, 20. We can realize that it is an increasing function of the parameter λ in the vicinity of the transition point. Additionally, we have plotted $dR^2/d\lambda$ at the transition point, and we can see that this function is always positive. Its slope goes to infinity in the thermodynamic limit $N \to \infty$. As we have said above the superradiant phase is degenerate in the thermodynamic limit, so , this result is valid in both normal (non-degenerate) and superradiant (degenerate) for $N \to \infty$ in accordance with theorem 4.

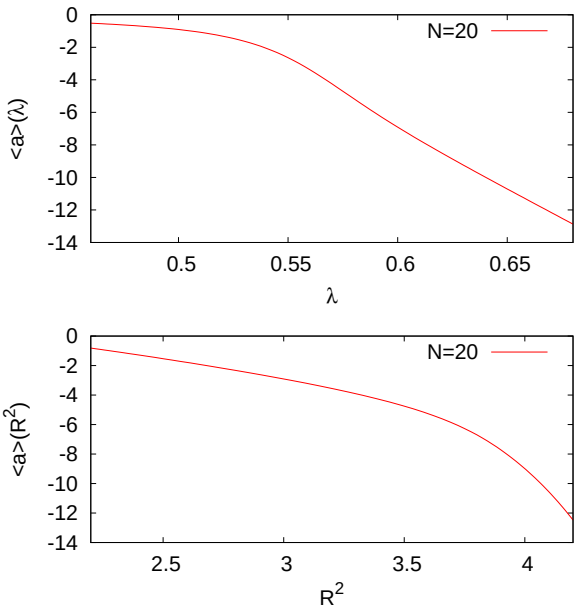

FIG. 2. (Color online) The 'subspace density' a as a function of (top) the parameter λ and (bottom) the Rényi entropy R^2, for $N = 20$, in the Dicke model and for $\omega_0 = \omega = 1$. (Atomic units).

In Fig. 2 (a) we have plotted the 'subspace density' $a = \langle \hat{A} \rangle$ and the 'external potential' λ. This behaviour is in accordance with theorem 2. In figure 2(b) we can see that there is a one-to-one map between the subspace density a and the Rényi information R^2 in the Dicke model (in agreement with Corollary 2).

Summarizing, we have studied via DFT a connection between the control parameter in a QPT and an analogous DFT subspace density in a ground state degenerate case. In particular (i) we have found that there is a one-to one map between the expectation value of a local function and the control parameter, and (ii) we have considered the Rényi entropies' case for which there is a one-to one map with the control parameters. Finally, we have illustrated these properties with the Dicke model which exhibits a QPT from a normal phase (non-degenerate) to a superradiant case (degenerate) in the thermodynamic limit.

APPENDIX

The ground state of the non-perturbed operator $\tilde{\hat{H}}_0$ is degenerate. The degenerate ground-state energy is $E_0^{(0)}$. Consider a unitary transformation of the original set of the nondegenerate basis functions. Let the new set Φ_γ

with $\gamma = 1, .., g$ so that using it as a basis diagonalizes the operator H' (Eq. (35)). The non-perturbed excited state eigenfunctions are denoted by $\Theta_{k,\kappa}$, $\kappa = 1, .., g_k$. Then the first-order correction to the ground-state wave function in Eq. (36) can be written as [34]

$$\Psi_\gamma^{(1)} = \sum_{k\neq 0}\sum_{\kappa=1}^{g_k}\sum_{\gamma'\neq\kappa}\Phi_{\gamma'}\frac{H'^*_{0,\kappa,\gamma'}H'_{k,\kappa,\gamma}}{(E_\gamma^{(1)}-E_{\gamma'}^{(1)})(E_0^{(0)}-E_k^{(0)})} + \sum_{k\neq 0}\sum_{\kappa=1}^{g_k}\Theta_{k,\kappa}\frac{H'_{k,\kappa,\gamma}}{E_0^{(0)}-E_k^{(0)}}, \quad (48)$$

where

$$E_\gamma^{(1)} = \langle\Phi_\gamma|H'|\Phi_\gamma\rangle, \quad (49)$$

subscript 0 and superscript 0 refer to the ground state and the unperturbed state, respectively and $H'_{k,\kappa,\gamma} \equiv \langle\Theta_{k,\kappa}|H'|\Phi_\gamma\rangle$. The first-order correction to the ground-state subspace density in Eq. (37) takes the form

$$\rho_1 = 2\sum_{\gamma=1}^{g} w_\gamma \mathrm{Re}[\Psi_\gamma^{(0)*}\Psi_\gamma^{(1)}] = 2\sum_{\gamma=1}^{g} w_\gamma \times \mathrm{Re}[\Psi_\gamma^{(0)*}\sum_{k\neq 0}\sum_{\kappa=1}^{g_k}\sum_{\gamma'\neq\kappa}\Phi_{\gamma'}\frac{H'^*_{0,\kappa,\gamma'}H'_{k,\kappa,\gamma}}{(E_\gamma^{(1)}-E_{\gamma'}^{(1)})(E_0^{(0)}-E_k^{(0)})} + \sum_{k\neq 0}\sum_{\kappa=1}^{g_k}\Theta_{k,\kappa}\frac{H'_{k,\kappa,\gamma}}{E_0^{(0)}-E_k^{(0)}}] \quad (50)$$

in case 1 (Eq. (39)). On the other hand, the first-order correction to the ground-state subspace density in Eq. (41) reads as

$$\rho_1 = 2\sum_{\gamma=1}^{g} w_\gamma \int dq \mathrm{Re}[\Psi_\gamma^{(0)*}\Psi_\gamma^{(1)}] = 2\sum_{\gamma=1}^{g} w_\gamma \times \int dq \mathrm{Re}[\Psi_\gamma^{(0)*}\sum_{k\neq 0}\sum_{\kappa=1}^{g_k}\sum_{\gamma'\neq\kappa}\Phi_{\gamma'}\frac{H'^*_{0,\kappa,\gamma'}H'_{k,\kappa,\gamma}}{(E_\gamma^{(1)}-E_{\gamma'}^{(1)})(E_0^{(0)}-E_k^{(0)})} + \sum_{k\neq 0}\sum_{\kappa=1}^{g_k}\Theta_{k,\kappa}\frac{H'_{k,\kappa,\gamma}}{E_0^{(0)}-E_k^{(0)}}] \quad (51)$$

in case 2 (Eq. (34)). Then we readily obtain the derivative of ω_α from Eq. (44).

If the degeneracy is not completely removed, another unitary transformation should be performed [35]. The new functions should be selected so that the matrix

$$t_{\gamma,\gamma'} = \sum_{k\neq 0}\sum_{\kappa=1}^{g_k}\frac{H'^*_{0,\kappa,\gamma'}H'_{k,\kappa,\gamma}}{E_0^{(0)}-E_k^{(0)}} \quad (52)$$

be diagonal. In this case the terms with zero in the denominator in Eq. (48) disappear and the sum can be obtained.

In the thermodynamic limit $E_k^{(0)} \to E_0^{(0)}$ for one or several values of k. It can be seen from Eqs. (50) and (51) that ρ_1 and therefore P, the derivative of ω_α and the derivative of the Rényi entropy diverge.

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