

A Density Functional Theory View of Quantum Phase Transitions

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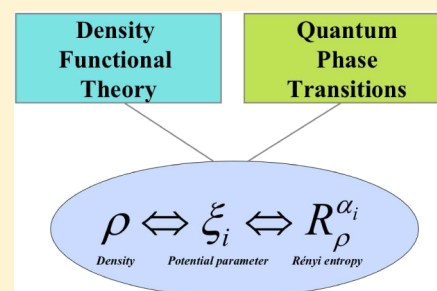
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ABSTRACT: It is shown that there is a one-to-one map between the ground state wave function and the control parameter. Wu et al. [*Phys. Rev. A* **2006**, *74*, 052335] introduced an analogue of the Density Functional Theory (DFT) density and showed that the “density” determines the “control parameter” (corresponding to the DFT “external potential”). We prove that any strictly monotonous function can be used to obtain a new density with a different control parameter (or DFT “external potential”), and the new density determines the new control parameter. Moreover, there is also a one-to-one map between the Rényi entropy of a given order and the control parameter. Therefore, the Rényi entropy can be used as a control parameter.



Quantum phase transitions (QPT)¹ have recently attracted increasing attention. QPT is an extension of classical phase transitions to quantum systems at zero temperature. In classical phase transitions, there is a change in the temperature that leads to an abrupt change in the physical properties of a system. In quantum phase transitions that occur at absolute zero of temperature, quantum fluctuations are responsible for a dramatic change in the properties of the system. Therefore, QPT is often described by variance and entropic uncertainty measures. It has also been shown that entanglement measures recognize QPT.

Density functional theory (DFT) is an approach applied frequently to obtain ground-state (or even excited-state) properties of systems. One of the relevant methods in determining ground-state energy and its derivatives is DFT. That is, density functional theory has its own right in studying QPT.

A couple of years ago, the density functional theory was generalized for quantum phase transition² in another aspect. In this paper, we extend the theory with the constrained search approach (see also refs 3–10 for related work on generalizing the mathematical structure of DFT to other variables with “extended constrained search” and “extended Legendre transform”). We prove that there is a one-to-one map between the ground state wave function and the control parameter. Wu et al.² introduced an analogue of the DFT density and showed that the “density” determines the control parameter (corresponding to the DFT “external potential.” We prove that any strictly monotonous function can be used to obtain a new “density” with a different “control parameter” (or DFT “external potential”), and the new “density” determines the new “control parameter.” Moreover, there is also a one-to-one map between the Rényi entropy of a given order and the control parameter. This fact makes it possible using the Rényi entropy as a control parameter.

In density functional theory, the ground-state electron density $\rho(\mathbf{r})$ is the fundamental quantity. According to the Hohenberg–Kohn theorems,¹¹ there is a one-to-one map between the density and the external potential $v(\mathbf{r})$. There exists a variational principle: for any trial density ρ , the energy is larger or equal to the exact ground-state energy. Equality stands only in the true ground state. Consider the Hamiltonian

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

where \hat{T} and \hat{V}_{ee} are the kinetic energy and the electron–electron energy operators, respectively. The total energy functional can be written as

$$E = F + \int \rho(\mathbf{r}) v(\mathbf{r}) d\mathbf{r} \quad (2)$$

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 2. It is defined only for those trial $\rho(\mathbf{r})$'s that are v -representable. A v -representable density is one that is associated with a ground-state wave function of some Hamiltonian with a local external potential. The conditions for a density to be v -representable are yet unknown. The v -representability problem was solved by the constrained search method of Levy and Lieb.^{12,13} A universal functional $F[\rho]$ is defined as $F[\rho] = \min_{\Psi \rightarrow \rho} \langle \Psi | \hat{T} + \hat{V}_{ee} | \Psi \rangle$. That is, the sum of the kinetic and electron energy is minimized subject to the constraint that each Ψ yield the given density ρ . The ground-state energy is searched in two steps:

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$$E_0 = \min_{\Psi} \langle \Psi | \hat{T} + \hat{V}_{ee} + \sum_{i=1}^N v(\mathbf{r}_i) | \Psi \rangle$$

$$= \min_n \{ \min_{\Psi \rightarrow n} \langle \Psi | \hat{T} + \hat{V}_{ee} | \Psi \rangle + \int v(\mathbf{r}) n(\mathbf{r}) d\mathbf{r} \} \quad (3)$$

The universal functional $F[\rho]$ can also be given as a Legendre transformation $F[\rho] = E - \int \rho(\mathbf{r}) v(\mathbf{r}) d\mathbf{r}$, where the electron density $\rho(\mathbf{r})$ becomes the fundamental quantity instead of the external potential $v(\mathbf{r})$. The functional derivative of F gives the external potential up to a constant

$$\frac{\delta F[n]}{\delta n} = -v(\mathbf{r}) \quad (4)$$

Consider now a quantum system with the Hamiltonian

$$\hat{H} = \hat{H}_0 + \sum_i \xi_i \hat{A}_i \quad (5)$$

where \hat{H}_0 is integrable and ξ_i represents the control parameters associated with \hat{A}_i . Note that \hat{H}_0 and \hat{A}_i are known Hermitian operators. The index i can be discrete or continuous [a continuous i (that is, a local function $\xi(\mathbf{r})$), with a local function $A(\mathbf{r})$, gives the original DFT]. Following Wu et al.,² we denote the expectation value of \hat{A}_i

$$a_i = \langle \Psi | \hat{A}_i | \Psi \rangle \quad (6)$$

According to the concept of constrained search, we construct the function

$$Q(\{a_i\}) = \min_{\Psi \rightarrow \{a_i\}} \langle \Psi | \hat{H}_0 | \Psi \rangle \quad (7)$$

that is, the expectation value of the Hamiltonian \hat{H}_0 is minimized subject to the constraint that each Ψ yields the given values a_i . Comparing with the original density functional theory, a_i corresponds to the density and ξ_i corresponds to the external potential.

The ground-state energy is searched in two steps:

$$E = \min_{\Psi} \langle \Psi | \hat{H} | \Psi \rangle = \min_{\{a_i\}} \{ \min_{\Psi \rightarrow \{a_i\}} \langle \Psi | \hat{H}_0 | \Psi \rangle + \sum_i \xi_i a_i \} \quad (8)$$

The total energy then has the form

$$E(\xi_1, \dots, \xi_M) = Q(a_1, \dots, a_M) + \sum_i \xi_i a_i \quad (9)$$

and Q can be considered as the Legendre transform of E

$$Q(a_1, \dots, a_M) = E - \sum_i \xi_i a_i \quad (10)$$

As Wu et al.² pointed out, the Hellmann–Feynman theorem leads to the result

$$\frac{\partial E}{\partial \xi_i} = \langle \Psi | \frac{\partial \hat{H}}{\partial \xi_i} | \Psi \rangle = \langle \Psi | \hat{A}_i | \Psi \rangle = a_i \quad (11)$$

Equations 10 and 11 lead to

$$\frac{\partial Q}{\partial a_i} = -\xi_i \quad (12)$$

Wu et al.² proved the Hohenberg–Kohn theorems: “for a nondegenerate ground state there is a one-to one map between the ‘density’ a_i and the ‘external potential’ $\{\xi_i\}$ and there holds the variational principle: the trial energy is always larger or

equal to the true ground-state energy with equality only for the true ground-state ‘density’ $\{a_i\}$.” Here, another proof based on the constraint search is presented. Only the nondegenerate case is considered here for the sake of simplicity, although these results could be extended to the nondegenerate case. First we prove the following:

Theorem 1. There is a one-to-one map between the nondegenerate wave function Ψ and the “external potential” $\{\xi_i\}$.

Proof: First, we prove that the “external potential” $\{\xi_i\}$ determines the wave function Ψ . If $\{\xi_i\}$ is known, the wave function Ψ can be readily obtained by solving the Schrödinger equation with the Hamiltonian (eq 5). Second, we have to prove that the nondegenerate wave function Ψ determines the “external potential” $\{\xi_i\}$; that is, only one “external potential” $\{\xi_i\}$ corresponds to a given Ψ . The proof proceeds by reductio ad absurdum. Suppose that there are two “external potentials” $\{\xi_i^{(1)}\}$ and $\{\xi_i^{(2)}\}$ with the same wave function Ψ . Then, the corresponding Schrödinger eqs 16 lead to

$$\sum_i (\xi_i^{(1)} - \xi_i^{(2)}) \hat{A}_i \Psi = (E^{(1)} - E^{(2)}) \Psi = \text{const. } \Psi \quad (13)$$

where $E^{(1)}$ and $E^{(2)}$ are the eigenvalues of the Hamiltonians $\sum_i \xi_i^{(1)} \hat{A}_i$ and $\sum_i \xi_i^{(2)} \hat{A}_i$, respectively. Equation 13 can also be written as $\hat{B} \Psi = 0$, where

$$\hat{B} = \sum_i (\xi_i^{(1)} - \xi_i^{(2)}) \hat{A}_i - (E^{(1)} - E^{(2)}) \quad (14)$$

Excluding the solution of $\Psi = 0$ (everywhere or in a domain of nonzero measure), the solution of $\hat{B} \Psi = 0$ is $\hat{B} = 0$, and it leads to $\xi_i^{(1)} = \xi_i^{(2)}$.

Note that the Hamiltonian (eq 5) can be reformulated as

$$\hat{H} = \hat{H}_0 + \sum_i \xi_i \hat{A}_i = \hat{H}_0 + \sum_i \zeta_i \hat{B}_i \quad (15)$$

where ζ_i represents the “new” control parameters associated with \hat{B}_i . The “new density” is defined by $b_i = \langle \Psi | \hat{B}_i | \Psi \rangle$. Certainly, there is a simple relationship between both parametrizations: $\hat{B}_i = \hat{A}_i \xi_i / \zeta_i$ and between a_i and $b_i = a_i \xi_i / \zeta_i$. Of course, $\zeta_i \neq 0$. As a direct consequence of the previous theorem, we have the following:

Corollary 1. If $\zeta_i = f_i(\xi_i)$ and f_i are strictly monotonous functions, there is a one-to-one map between the nondegenerate wave function Ψ and the “external potential” $\{\xi_i\}$.

Theorem 2. There is a one-to one map between the “density” a_i and the “external potential” $\{\xi_i\}$.

Proof: If $\{\xi_i\}$ is known, $\{a_i\}$ can be readily obtained by solving the Schrödinger equation with the Hamiltonian (eq 5) and calculating the expectation values (eq 6). On the other hand, $\{\xi_i\}$ can also be determined in the knowledge of $\{a_i\}$. First, the wave function Ψ should be found by minimizing the expectation value of the Hamiltonian \hat{H}_0 subject to the constraint that each Ψ yields the given values a_i (see eq 7). Knowing Ψ , we have to find $\{\xi_i\}$ for which Ψ fulfills the Schrödinger equation

$$\hat{H} \Psi = (\hat{H}_0 + \sum_i \xi_i \hat{A}_i) \Psi = E \Psi \quad (16)$$

A consequence of theorem 2 is that we can use the “density” $\{a_i\}$ as fundamental variable instead of the “external potential” $\{\xi_i\}$; that is, $\{a_i\}$ can play the role of the control parameter.

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 “density” b_i and the “external potential” $\{\zeta_i\}$.

Theorem 3. The following inequality holds:

$$Q(a_1, \dots, a_M) + \sum_i \xi_i a_i \geq E_{\text{gs}} \quad (17)$$

where E_{gs} is the ground-state energy of the Hamiltonian H of eq 5. Equality holds if and only if $\{a_i\}$ is the ground-state “density.”

Proof: The proof was given above in the constrained search approach [see eqs 7 and 8].

Corolary 3. The following inequality holds:

$$Q(b_1, \dots, b_M) + \sum_i \zeta_i b_i \geq E_{\text{gs}} \quad (18)$$

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

The Rényi entropy is defined as

$$R^\alpha = \frac{1}{1-\alpha} \ln \int \rho^\alpha(q) dq \quad (19)$$

where $\alpha > 0$ and $\rho = |\Psi|^2$ is the normalized density.

Theorem 4. The Rényi entropy R^α of the ground state density $\rho_0(x) = |\psi_0(x)|^2$ 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: Without a loss of generality, we shall consider a single control parameter ξ . First, we shall write the Hamiltonian in terms of a new parameter $\lambda = \xi - \xi_c$:

$$\hat{H} = \hat{H}_0 + \lambda \hat{H}' \quad (20)$$

with $\hat{H}_0 = \hat{H} + \xi_c \hat{A}$ and $\hat{H}' = \hat{A}$. We will prove that $\omega_\alpha \equiv \int \rho_\alpha^\alpha(x) dx$ is a strictly monotonous function of λ in a neighborhood of $\lambda = 0$. Then, it is straightforward to see that the Rényi entropy R^α has the same monotonic behavior, because the logarithm is an increasing function. A non-degenerate ground state ψ_0 is considered. In perturbation theory, the ground state wave function ψ_0 can be written in terms of the nonperturbed wave functions $\psi_0^{(0)}$ as

$$\psi_0 = \psi_0^{(0)} + \lambda \sum_{m \neq 0} \frac{H'_{m0}}{E_0^{(0)} - E_m^{(0)}} \psi_m^{(0)} + O(\lambda^2) \quad (21)$$

where the superscript (0) refers to the nonperturbative eigenfunctions and eigenenergies. Making use of the McLaurin expansion of the function $f(y) = (a + y)^\alpha$, we can write

$$\omega_\alpha(\lambda) = \omega_\alpha^{(0)} + \lambda \alpha A + O(\lambda^2) \quad (22)$$

with

$$A = \sum_{m \neq 0} \frac{H'_{m0}}{E_0^{(0)} - E_m^{(0)}} \int \rho_0^{(0)}(x)^{\alpha-1} 2\text{Re}[\bar{\psi}_0^{(0)}(x) \psi_m^{(0)}(x)] dx \quad (23)$$

and $\omega_\alpha^{(0)}$ independent of λ . Thus, we have that $d\omega_\alpha(0)/d\lambda = \alpha A$. On the one hand, A is nonzero (either strictly positive or negative), and therefore, $\omega_\alpha(\lambda)$ is strictly monotonous in a neighborhood of $\lambda = 0$. It is obvious that, in the thermodynamic limit (that is, when $E_m^{(0)} \rightarrow E_0^{(0)}$ for one or several values of m), A diverges (as one expects for a step function $\omega_\alpha(\lambda)$ at $\lambda = 0$).

Two particular cases could be of special interest: the case $\alpha=1$ for which the Rényi entropy is the Shannon entropy $R^1 = -\int \rho \ln \rho$ and the case $\alpha \rightarrow \infty$ for which the Rényi entropy is given by $R^\infty = \max_x \{\ln \rho(x)\}$.

Corolary 4. As the Rényi entropies R^α are strictly monotonous functions of $\{\xi_i\}$ 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” $\{\xi_i\}$.

As an illustration, the vibron model is considered. Vibron models were constructed to study rotational and vibrational spectra in diatomic and polyatomic molecules. These models, introduced by Iachello,¹⁴ exhibit a (shape) QPT. Consider the two-dimensional $U(3)$ vibron model of a system with a dipole degree of freedom for planar motion. 2D-vibron models^{14–17} can be constructed with a τ vector boson and a σ scalar boson. The creation and annihilation operators are $\tau_x^\dagger, \tau_y^\dagger, \tau_x, \tau_y$, and σ^\dagger, σ , respectively. Using “circular” bosons, $\tau_\pm = (\tau_x \mp i\tau_y)/\sqrt{2}$, the nine generators of the $U(3)$ algebra can be expressed as bilinear products of creation and annihilation operators. For example, we shall consider

$$\hat{n} = \tau_+^\dagger \tau_+ + \tau_-^\dagger \tau_-, \quad \hat{l} = \tau_+^\dagger \tau_+ - \tau_-^\dagger \tau_-, \quad \hat{n}_\sigma = \sigma^\dagger \sigma, \quad \hat{D}_\pm = \sqrt{2}(\pm \tau_\pm^\dagger \sigma \mp \sigma^\dagger \tau_\pm) \quad (24)$$

The remaining four operators (\hat{Q}_\pm, \hat{R}_\pm) are not important here (see ref 17). The total number operator $\hat{N} = \hat{n} + \hat{n}_\sigma$ and the 2D angular momentum operator \hat{l} being conserved leads to two dynamical symmetry limits: the $U(2)$ (cylindrical) and the $SO(3)$ (displaced oscillator) chains.¹⁷ Our quantum system can now be described by the “essential” Hamiltonian¹⁷

$$\hat{H} = (1 - \xi)\hat{n} + \xi \frac{N(N+1) - \hat{W}^2}{N-1} \quad (25)$$

where $\hat{W}^2 = (\hat{D}_+ \hat{D}_- + \hat{D}_- \hat{D}_+)/2 + \hat{l}^2$ is the quadratic $C_2(SO(3))$ Casimir operator (the squared angular momentum) and $\xi \in [0,1]$ is the control parameter. The Hamiltonian of the vibron model can be rewritten (in the form of eq 5) as $\hat{H} = \hat{H}_0 + \xi \hat{A}$, where

$$\hat{H}_0 = \hat{n}, \quad \hat{A} = -\hat{n} + \frac{N(N+1) - \hat{W}^2}{N-1} \quad (26)$$

The (constant) quantum number N (the eigenvalue of the linear Casimir \hat{N}) is the total number of bound states that labels the totally symmetric $(N+1)(N+2)/2$ -dimensional representation $[N]$ of $U(3)$. This model exhibits a (shape) QPT at $\xi_c = 0.2$.¹⁷ The Hamiltonian (eq 25) has been numerically diagonalized (see more details in refs 18, 19, and 20 for other delocalization measures in the vibron model and in the Dicke model^{21,22}). Figure 1 presents the Rényi entropy $R^2(\xi)$ and its derivative as a function of the parameter ξ for different values of $N = 6, 12$, and 24 . As has been shown in ref 18, Rényi entropy detects the quantum (shape) phase transition (from linear to bent) at the critical value of the control parameter. Figure 1 is in accordance with theorem 0, showing that the Rényi entropies are strictly monotonous (increasing in this case) functions of the control parameter ξ in the vicinity of the transition point $\xi_c = 0.2$ and that their slope grows at ξ_c as N (the size of the system) increases, going to infinity in the thermodynamic $N \rightarrow \infty$ limit.

The “density” a is given by the expectation value of the operator \hat{A} in eq 26. Figure 2 shows the “density” a as a function of ξ and as a function of Rényi entropy R^2 . According

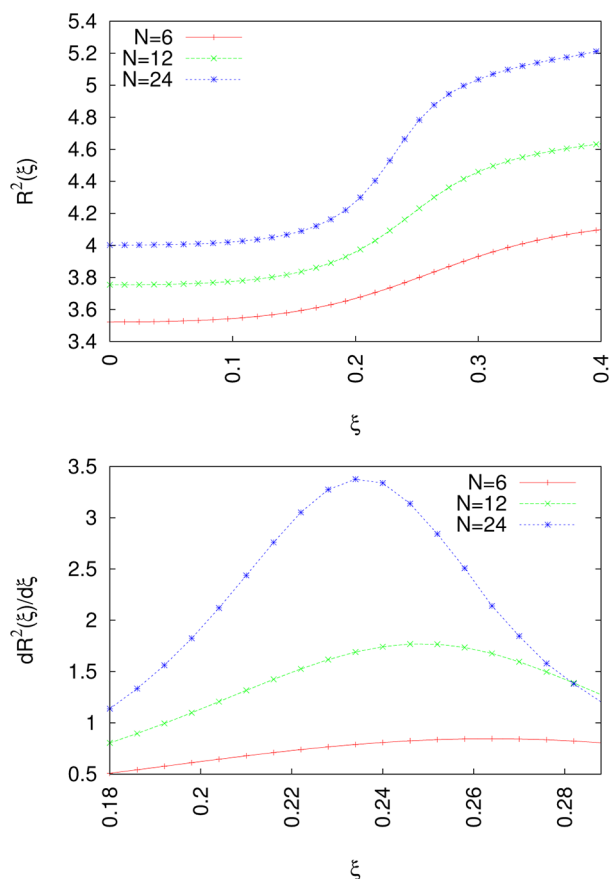


Figure 1. Rényi entropy $R^2(\xi)$ (top) and its derivative $dR^2(\xi)/d\xi$ (bottom) as a function of the control parameter ξ for different values of $N = 6, 12$, and 24 in the vibron model. Dimensionless units.

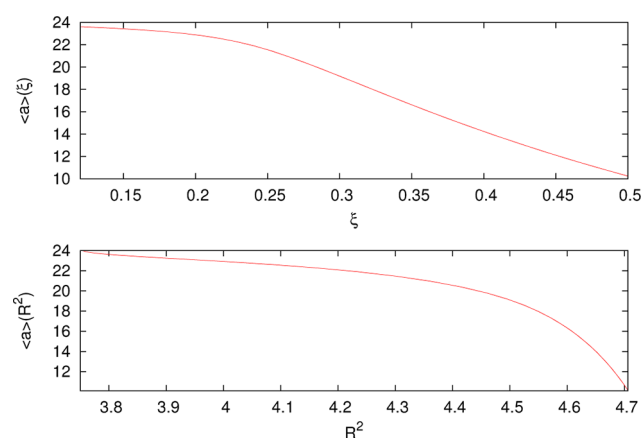


Figure 2. The “density” a as a function of (top) the parameter ξ and (bottom) the Rényi entropy R^2 , for $N = 24$, in the vibron model. Dimensionless units.

to corollary 4, the Rényi entropy can also be considered as a “control parameter” and could also be plotted against the “density” a .

In the thermodynamic or mean-field $N \rightarrow \infty$ limit, Gilmore²³ applied semiclassical (boson-condensate) Coherent States (CSs) as variational states. The CS contains a variational parameter r that can be determined by minimizing the mean energy per particle:¹⁷ $\partial E_\xi(r)/\partial r = 0 \Rightarrow r = r_c(\xi)$. The second derivative $d^2E(\xi)/d\xi^2$ of the minimum mean energy $E(\xi) = E_\xi(r_c(\xi))$ is discontinuous at $\xi_c = 0.2$; therefore, the phase

transition is of second order. Expressions in ref 17 lead to the “density” a as a function of the “external potential” ξ : $a/N = 1$ if $\xi \leq \xi_c = 1/5$ and $a/N = (1 - 9\xi^2)/(16\xi^2)$ if $\xi > \xi_c = 1/5$. This result can also be obtained from eq 11 [see also Figure 11b in ref 17]. As described above, we can use a instead of ξ . However, a/N is constant if $\xi \leq \xi_c = 0.2$. Thus, the procedure above leads to incorrect results. It has already been pointed out that the results above are correct except in the thermodynamic limit $N \rightarrow \infty$. Here, we provide another reason that it cannot be correct.

The importance of using the “density” a instead of the “external potential” ξ as a basic variable lies in the fact that in a phase transition this “density” a is especially important, as it is related to the order of the transition. In a first order QPT, there is a finite discontinuity in the first derivative of the ground-state energy, that is in the “density” a . In a second-order QPT, there is a finite discontinuity or divergence in the second derivative of the ground-state energy, that is in the first derivative of the “density” a . Therefore, the “density” a is a good indicator of QPT.

Though the theory presented here is very similar to DFT, there is an important difference. In DFT, we have a local external potential, and the density is also a function. Here, a and ξ are numbers. The similarity is based on the fact that the Hamiltonian has a given fixed form in both theories. In the constrained search approach, the operators \hat{T} and \hat{V}_{ee} are known. Similarly, the fact that the operators in eq 5 have fixed known forms is used in the above derivation.

According to the original Hohenberg–Kohn theorems,¹¹ the density determines the external potential up to a constant. In the theory described here, we have a freedom in selecting the control parameter (ξ or ζ), that is, the “external potential.” (Of course, the definition of the “density” is related to the selection of the “external potential.”)

In summary, quantum phase transitions are considered from a DFT aspect. In a nondegenerate ground state, there exists an analogue of the DFT density, and this “density” determines the control parameter (corresponding to the DFT “external potential”). It is proved that any strictly monotonous function can be used to obtain a new “density” with a different “control parameter” (or DFT “external potential”), and the new “density” determines the new “control parameter.” As the Rényi entropy of a given order is a strictly monotonous function of the control parameter in the vicinity of the transition point, the Rényi entropy can also play the role of the control parameter.

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Notes

The authors declare no competing financial interest.

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