Ground-state-energy universality of noninteracting fermionic systems

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When noninteracting fermions are confined in a *D*-dimensional region of volume $O(L^D)$ and subjected to a continuous (or piecewise-continuous) potential *V* which decays sufficiently fast with distance, in the thermodynamic limit, the ground-state energy of the system does not depend on *V*. Here, we discuss this theorem from several perspectives and derive a proof for radially symmetric potentials valid in *D* dimensions. We find that this universality property holds under a quite mild condition on *V*, with or without bounded states, and extends to thermal states. Moreover, it leads to an interesting analogy between Anderson's orthogonality catastrophe and first-order quantum phase transitions.

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I. INTRODUCTION AND MAIN RESULT

Noninteracting systems represent a crucial limit where analytic solutions are possible and provide the zeroth-order insight into the understanding of more realistic models. In particular, noninteracting systems can be analyzed in the thermodynamic limit (TDL), which provides a dramatically important link between theoretical models (microscopic) and experiments (macroscopic). In fact, the TDL is defined as the limit where both the number of particles and the volume diverge while keeping their ratio constant.

The main result we are going to discuss in this work concerns the TDL of the ground-state (GS) energy of noninteracting fermionic systems confined in some "box." Let us consider a system of N noninteracting fermions confined in a compact region of volume proportional to L^{D} , where L is the length and D is the dimensionality of the space considered. The corresponding one-particle stationary Schrödinger equation must be solved with Dirichlet boundary conditions, i.e., imposing that the eigenfunctions are zero at the boundaries of the box (box with rigid walls). Let E(N, L) be the GS energy of this system. Let us consider then another system of N noninteracting fermions confined in the same box as in the previous system with the same boundary conditions but suppose that, now, the fermions are subjected also to an external potential V. Let us indicate by $\tilde{E}(N, L)$ the GS energy of this second system. The general result we want to discuss is that, for L large, the GS energies of these two systems differ at most by o(L) terms or, in other words, that in the TDL limit, where both the GS energies (which are extensive observables) diverge as $O(L^D)$, their ratio tends to 1. More precisely, for a spherically symmetric continuous (or, more generally, piecewise-continuous) potential V(r), where r is the radial distance, that satisfies the condition on the radial integral

$$\int_0^L V(r)dr = O(L^{1-\alpha}), \quad \alpha > 0, \tag{1}$$

we have

$$\tilde{E}(N,L) = E(N,L) + O(\rho L^{D-\alpha}), \qquad (2)$$

which, by using $E(N, L) = O(L^D)$, provides

$$\lim_{N \to \infty, L \to \infty, N/L^D = \rho} \frac{\tilde{E}(N, L)}{E(N, L)} = 1,$$
(3)

where $\rho = N/L^D$ stands for the particle density. Alternatively, Eq. (3) can be restated by saying that, in the TDL, the GS energy per particle of the two systems is the same, and in particular, it depends on the boundary conditions but not on V (it is usually assumed that the boundary conditions do not matter in the TDL, which is true if $\alpha > D$, as proved rigorously in [1], as well as if $\alpha = D$, as proved rigorously in [2]; however, for $\alpha < D$, no proof exists, and boundary conditions might matter). In other words, at zero temperature, given the boundary conditions and the particle density, we have the universality of the energy density. Moreover, we shall show that, in the case in which the integral in Eq. (1) is negative, the number of eigenstates with negative energy N_0 turns out to be nonextensive and scales as

$$N_0 = O(L^{D(1-\alpha/2)}), (4)$$

whereas $N_0 = 0$ if $V \ge 0$ or, at most, $N_0 = O(1)$ when the integral in Eq. (1) is positive.

It is not hard to verify that Eq. (2) is consistent with the Lieb-Thirring inequalities in a box [3], which provide rigorous bounds to the GS energy of a perturbed ideal gas via terms corresponding to the "semiclassical approximation." However, the results in [3] do not cover the case D = 1since the semiclassical approximation there suffers from the presence of a Fermi-edge singularity [4]. Our simple, but general, result is valid also for D = 1 and unifies in a single group of scaling laws all the cases, including the cases with $\alpha \leq D$, i.e., the cases where the volume integral of the potential diverges in the TDL. In particular, Eqs. (2) and (4) show the following: Whereas the energy shift caused by the potential diverges for $L \to \infty$ (although not extensively) only when $\alpha < \alpha_E = D$, the threshold value for N_0 is $\alpha_0 = 2$, independent of D. This implies that, for any given D, we can design experiments where the thermodynamic properties of the system with the potential are indistinguishable from those without the potential and yet, unlike the latter, the former contains states that remain bounded in the TDL (although in a nonextensive manner). In other words, we can accommodate an infinite number of electrons such that they are bounded around the minima of V and still have a system that as a whole behaves as a perfect gas of fermions (and we can design such an experiment regardless of D, provided $\alpha < 2$).

As the next section will make evident, at the base of the above universality lie two facts: the absence of interaction and the exclusion principle. As is well known, the latter is the essential key for the stability of matter, as stressed long ago by Lieb in his monumental work [2]. It is worth mentioning, however that, despite the obvious simpler nature of noninteracting systems, their universality, in the sense of the Lieb-Thirring inequalities or in the sense of Eq. (3), emerged only recently. In fact, the Lieb-Thirring inequalities in a box are the result of a formidable mathematical *tour de force* that only experts in the spectral theory of Hilbert spaces are capable of following. Here, we use a quite simpler strategy that allows us to tackle also the D = 1 case.

The proof for D = 1 is based on a Prüfer-variables setting already used in [5], which inspired us also to prove the cases D = 2 and D = 3. As a technical note, we observe that in [5] (and references therein), formulas for the difference in the GS energies $\tilde{E}(N,L) - E(N,L)$ are expressed in terms of integrals of the spectral shift function for oneparticle Schrödinger operators. The concept of the spectral shift function is common in the spectral theory of Hilbert spaces [6,7] and in the foundations of Anderson's orthogonality catastrophe (AOC) [8] discussed, in particular, in [9,10]; however, except for a Dirac- δ potential V, the formulas for the spectral shift function turn out to be quite involved and hard to handle. In particular, it seems very difficult to control the order of magnitude of the spectral shift function with respect to N and L in the TDL, which is crucial for proving Eq. (3). An exception is the case D = 1, where in [5] useful bounds for the spectral shift function are explicitly worked out and used to express the GS-energy difference in detail, which, in particular, implies Eq. (3). This result of Ref. [5] is, however, obtained under the condition that $\int_0^L V(r)r^2 dr < 1$ ∞ , which represents a much more stringent condition than Eq. (1).

Here, we show how to deal with the cases D = 1, 2, and 3 in a simpler way that does not make use of the spectral shift function (for convenience, the D = 2 case is discussed after the D = 3 case). We start demonstrating the general result (3) by using an intuitive heuristic argument that, at the same time, shows why Eq. (3) cannot hold for bosons. We then produce formal proofs and finally show how Eq. (3) suggests an interesting analogy between AOCs and first-order quantum phase transitions [11]. Examples as well as counterexamples which show that Eq. (1) constitutes a necessary and sufficient condition are presented in the Appendix.

II. HEURISTIC ARGUMENT

Let us consider a *D*-dimensional box of volume L^D with hard walls and N noninteracting fermions subjected to a potential V with compact support over a region of volume ℓ^{D} . Since the box has hard walls, the wave function of each fermion must be zero outside the box. Moreover, the Pauli principle implies that the GS energy is the sum of the first N single-particle energies (accounting for their possible degeneracies; note that, for simplicity, we assume spinless fermions, but if $D \ge 2$, the single-particle energies may have degeneracies in the quantum numbers of the angular momentum). Consider now a sequence of boxes of increasing volumes L_1^D, L_2^D, \ldots and a corresponding number of fermions N_1, N_2, \ldots , such that the ratio $\rho = N_i/L_i^D$, $i = 1, 2, \ldots$, is kept constant. For a sufficiently large index i we will have $\ell < L_i$ and, eventually, $\lim_{i\to\infty} \ell/L_i = 0$. On the other hand, for $\ell \ll L_i$ the contribution of V to the single-particle energies will be $O(\ell/L_i)$, at least for those levels, corresponding to a sufficiently large radial quantum number, for which the particles are, on average, homogeneously distributed in the box. All these elements allow us to conclude that the GS energy of the system in the presence of V becomes closer and closer to that of the pure box when N and L are larger and larger, which is equivalent to Eq. (3). It is easy to guess that the condition that V has a fixed compact support can be relaxed. In fact, in the formal derivation we shall show that the necessary and sufficient condition is the quite mild one provided in Eq. (1).

The above heuristic argument also makes it evident that there is no analog of Eq. (3) for noninteracting bosons. In fact, their GS corresponds to a condensate in the lowest-energy single-particle state, which implies that the particles distribute near the region where V is minimum.

III. PROOF OF EQUATIONS (1)–(4) USING PRÜFER'S VARIABLES

In the Appendix, we consider explicit examples and show how Eq. (3) realizes when V is given by one or two Dirac- δ functions, and it is plausible that similar results hold for any number of Dirac- δ functions. Since any potential V can be approximated by a suitable sum of Dirac- δ functions, eventually, in an infinite number, in principle, one could attempt a general derivation of Eq. (3) extending the above results. However, it seems technically very hard to generalize the involved algebra to any number of Dirac δ 's, and we prefer to resort to a different strategy based on the Prüfer variables [12], which is a common tool within the Sturm-Liouville theory [1].

We suppose that V is piecewise continuous throughout the compact region defining a box of side L with rigid walls and assume the validity of Eq. (1). Note that these conditions, besides implying the existence and regularity of the eigenfunctions of the Schrödinger equation for any L [1], imply also that the number of eigenstates with negative energy N_0 (if any) is finite for any L and, as we shall see below, remains nonextensive in the TDL; that is, such eigenstates give no net contribution to the GS, namely, the general result (4). Therefore, unless explicitly stated otherwise, in the following we shall focus on only positive eigenvalues.

A. D = 1

Consider the following two eigenvalue problems:

$$-\frac{d^2u}{dr^2} = k^2 u, \quad u(0) = u(L) = 0,$$
(5)

$$-\frac{d^2u}{dr^2} + \mathcal{V}u = \tilde{k}^2 u, \quad u(0) = u(L) = 0, \tag{6}$$

where $\mathcal{V} = (2m/\hbar^2)V$ and k and \tilde{k} are real, i.e., we look for positive eigenenergies $E = \hbar^2 k^2/2m$ and $\tilde{E} = \hbar^2 \tilde{k}^2/2m$, respectively. Concerning Eq. (5), the eigensolutions are given by $u = A \sin(kr)$, and the boundary conditions imply the "infinite-square-well" values $k = n\pi/L$, with *n* being a nonnull integer. Concerning Eq. (6), following [5], we introduce implicitly the Prüfer variables, ρ and θ , by making the following ansatz:

$$u(r) = \rho(r) \sin[\theta(r)], \tag{7}$$

$$u'(r) = \tilde{k}\rho(r)\cos[\theta(r)].$$
(8)

The physical idea of the above ansatz is that, when $V \rightarrow 0$, the ansatz works with $\rho \rightarrow \text{const}$, $\theta(r) \rightarrow kr$, and $\tilde{k} \rightarrow n\pi/L$, while, for $V \neq 0$, ρ is not constant, $\theta(r)$ is not linear in r, and $\tilde{k} \neq n\pi/L$ but, in general, $\delta = \theta(r) - \tilde{k}r$ (which provides the so-called phase-shift scattering) will somehow be small, hence rendering the ansatz effective. By making use of Eqs. (7) and (8) we see that Eq. (6) is equivalent to the following system of first-order (ODE)

$$\rho' = \frac{1}{\tilde{k}} \mathcal{V}(r) \sin[\theta(r)] \cos[\theta(r)]\rho(r), \quad \rho(r) > 0, \quad (9)$$

$$\theta' = \tilde{k} - \frac{1}{\tilde{k}} \mathcal{V}(r) \sin^2[\theta(r)], \quad \theta(0) = 0, \quad \sin[\theta(L)] = 0.$$

(10)

Although the above first-order system is not useful for solving for u (in fact, it is even nonlinear), it offers the best way to compare \tilde{k} and k with each other, which is our main aim. Let us integrate Eq. (10) between r = 0 and r = L. By using the boundary conditions we get $\theta(L) = n\pi = k_n L$ and obtain

$$\tilde{k}_n = k_n + \frac{1}{L\tilde{k}_n} \int_0^L dr \mathcal{V}(r) \sin^2[\theta_n(r)], \quad n = 1, \dots, N,$$
(11)

where we have inserted the dependences on the integer index n of the eigenvalues running from 1 to the number of particles N. Since we are dealing with spinless fermions, for any such quantum numbers n we can allocate only one fermion. Up to this point, we have followed [5], where Eq. (11) is used to grasp the O(1/L) corrections of the GS energy in a sophisticated manner, where the O(1/L) terms are related to the decay exponent of the AOC. Here, we follow a less demanding and simpler strategy which is enough for our aims. Let us rewrite Eq. (11) as an equation for the eigenenergy \tilde{E}_n as a function of E_n . After multiplying by \tilde{k}_n and squaring the equation we get

 $\tilde{E}_n^2 - (E_n + 2b)\tilde{E}_n + b^2 = 0,$ (12)

where

$$b = \frac{1}{L} \int_0^L V(r) \sin^2[\theta_n(r)] dr.$$
(13)

For simplicity, in *b* we have dropped a harmless dependence on *n*. The important point to observe is that, under the condition (1), we have $b = O(1/L^{\alpha})$ for some $\alpha > 0$. The roots of Eq. (12) are

$$\tilde{E}_n = \frac{1}{2}E_n + b \pm \frac{1}{2}\sqrt{E_n^2 + 4bE_n}.$$
(14)

Note that, if b < 0, for some *n* the roots \tilde{E}_n may not be real. When this occurs, it simply means that \tilde{E}_n is actually negative, against our initial assumption. However, by using $E_n^2 = O(n^4/L^4)$ and $bE_n = O(n^2/L^{2+\alpha})$, we see that, if b < 0, the number N_0 of eigenstates with negative energy scales as $N_0 = O(L^{1-\alpha/2})$. This implies that, as anticipated, the condition (1) being negative implies $N_0/N \to 0$, i.e., a nonextensive N_0 . As a worst-case example where $\alpha = 0$, consider a piecewise constant potential taking the value $V(r) = V_0 < 0$ over a fractional portion of the box fL, with 0 < f < 1, and V(r) = 0 elsewhere. In this case we obtain $N_0 \simeq \sqrt{2fm|V_0|L^2/\hbar^2}$, in agreement with known general results [13].

Taking into account that the final target is to sum over n = 1, ..., N in the TDL, with $N/L = \rho$ being constant, and by using again $E_n^2 = O(n^4/L^4)$ and $bE_n = O(n^2/L^{2+\alpha})$, we see that in the square root of Eq. (14) we can neglect the last term except for a number of low-energy levels, which scales as N_0 , i.e., which can be disregarded in the TDL. Finally, choosing the root that is consistent with the limit $V \rightarrow 0$, we arrive at

$$\tilde{E}_n = E_n + 2b + \ldots = E_n + O\left(\frac{1}{L^{\alpha}}\right), \quad (15)$$

which implies

$$\tilde{E}(N,L) = E(N,L) + O(\rho L^{1-\alpha})$$
(16)

and then Eq. (3).

Above, we have actually used an asymptotic expansion which might not sound rigorous. However, we can use rigorous bounds as follows. First, observe that from the positive root of Eq. (14) we have

$$\tilde{E}_n \leqslant E_n + 2b. \tag{17}$$

On the other hand, if we now assume that $b \ge 0$, which in general does not prevent the potential V from taking some negative values, we also have

$$\tilde{E}_n \geqslant E_n + b. \tag{18}$$

Equations (17) and (18) imply $b \leq \tilde{E}_n - E_n \leq 2b$, leading again to Eq. (16).

B. D = 3

In three dimensions, we express the Laplacian in spherical coordinates and assume spherical boundary conditions and a spherical symmetric potential V = V(r). Given a spherical harmonic Y_l^m with total angular momentum l and magnetic momentum m, the eigenvalue equations for the radial part of the wave function R(r) written in terms of the function

u(r) = rR(r) read like Eqs. (5) and (6) augmented with the "centrifugal contribution":

$$-\frac{d^2u}{dr^2} + \frac{l(l+1)u}{r^2} = k^2u, \quad u(0) = u(L) = 0, \quad (19)$$

$$-\frac{d^2u}{dr^2} + \mathcal{V}u + \frac{l(l+1)u}{r^2} = \tilde{k}^2 u, \quad u(0) = u(L) = 0, \quad (20)$$

where, as before, k and \tilde{k} are real, i.e., we look for positive eigenenergies $E = \hbar^2 k^2 / 2m$ and $\tilde{E} = \hbar^2 \tilde{k}^2 / 2m$, respectively. Concerning Eq. (19), the eigensolutions are given by the Bessel functions $u = A j_l(kr)$, and the boundary conditions are satisfied by their zeros, which are different from k = $n\pi/L$. However, it is not necessary to make use of the Bessel functions as we can work out the D = 3 case by using the previous setting of the Prüfer variables with suitable modifications as follows. On comparing Eqs. (19) and (20) with Eqs. (5) and (6), we see that we cannot simply replace \mathcal{V} with $\mathcal{V} + l(l+1)/r^2$ and repeat the D = 1 argument since the centrifugal term produces a diverging integral. Nevertheless, we can integrate the analog of Eq. (10) between some fixed $\epsilon > 0$ and L and at the end send ϵ to zero suitably to satisfy the lower boundary condition $\theta(0) = 0$. We have to do this for the cases both with and without V. Note that, now, the Prüfer variable θ refers to the case with V = 0, while for the case with $V \neq 0$ we use the symbol $\tilde{\theta}$. We have

$$n\pi - \theta_n(\epsilon) = k_n(L - \epsilon)$$
$$- \frac{1}{k_n} \int_{\epsilon}^{L} dr \frac{l(l+1)}{r^2} \sin^2[\theta_n(r)], \qquad (21)$$

$$n\pi - \theta_n(\epsilon) = k_n(L - \epsilon)$$
$$- \frac{1}{\tilde{k}_n} \int_{\epsilon}^{L} dr \left[\mathcal{V}(r) + \frac{l(l+1)}{r^2} \right] \sin^2[\tilde{\theta}_n(r)],$$
(22)

which gives

$$\tilde{k}_{n} = k_{n} + \frac{1}{(L-\epsilon)\tilde{k}_{n}} \int_{\epsilon}^{L} dr \left[\mathcal{V}(r) + \frac{l(l+1)}{r^{2}} \right] \sin^{2}[\tilde{\theta}_{n}(r)] - \frac{1}{(L-\epsilon)k_{n}} \int_{\epsilon}^{L} dr \frac{l(l+1)}{r^{2}} \sin^{2}[\theta_{n}(r)] + \frac{\theta_{n}(\epsilon) - \tilde{\theta}_{n}(\epsilon)}{L-\epsilon}.$$
(23)

We find it convenient to rewrite the above expression as follows:

$$\tilde{k}_{n} = k_{n} + \frac{1}{(L-\epsilon)\tilde{k}_{n}} \int_{\epsilon}^{L} dr \mathcal{V}(r) \sin^{2}[\tilde{\theta}_{n}(r)] + \frac{l(l+1)}{(L-\epsilon)\tilde{k}_{n}} \int_{\epsilon}^{L} dr \frac{1}{r^{2}} \bigg[\sin^{2}[\tilde{\theta}_{n}(r)] - \frac{\tilde{k}_{n}}{k_{n}} \sin^{2}[\theta_{n}(r)] \bigg] + \frac{\theta_{n}(\epsilon) - \tilde{\theta}_{n}(\epsilon)}{L-\epsilon}.$$
(24)

Note that the dependence on *n* inside the square brackets of the integrand of the third term is weak and negligible with respect to the dependences on *n* of \tilde{k}_n and k_n . We can now choose ϵ as a suitable function of *L* such that $\epsilon(L) \rightarrow 0$ for

 $L \to \infty$, and the third term becomes infinitesimal in the TDL. For example, we can choose $\epsilon(L) = d/L^{1-\delta}$, with $1 > \delta > 0$ and *d* being constant. In this way the third term becomes $O(l^2/(\tilde{k}_n L^{\delta}))$. Note also that, for $L \to \infty$, the fourth term on the right-hand side of Eq. (24) goes to zero faster than the third one because both $\theta_n(\epsilon)$ and $\tilde{\theta}_n(\epsilon)$ tend to $n\pi$. Therefore, we can repeat the same steps as in Eqs. (12)–(14) and reach the same conclusions, with the only difference being that, now, $b = O(1/L^{\alpha}) + O(l^2/L^{\delta})$. The fact that $\delta > 0$ here is any arbitrary positive number, at most 1, just means that, as soon as l > 0, if $\alpha = 0$, the centrifugal term provides the leading correction to the GS energy; otherwise, we choose $\delta = \alpha$, so that the two corrections become equally dominant. In either case, we are left with Eq. (2).

C. D = 2

In two dimensions, we express the Laplacian in polar coordinates and assume circular boundary conditions and a symmetric potential V = V(r). After separating the variables, the eigenvalue problems for the radial part of the wave function become

- 2

$$-\frac{d^{2}u}{dr^{2}} + \frac{1}{r}\frac{du}{dr} + \frac{m^{2}u}{r^{2}} = k^{2}u, \quad u(0) = u(L) = 0, \quad (25)$$
$$-\frac{d^{2}u}{dr^{2}} + \frac{1}{r}\frac{du}{dr} + \frac{m^{2}u}{r^{2}} + \mathcal{V}u = \tilde{k}^{2}u, \quad u(0) = u(L) = 0, \quad (26)$$

where the integer *m* is the quantum number of the angular momentum. Note that, unlike the cases with D = 1 (the infinite square well plus some potential) and D = 3 (where u/rrepresents the radial part of the wave function), for D = 2 the boundary condition at r = 0 does not need to be zero [note that here u(r) is the true radial part of the wave function]. We could, in fact, choose any other value and reach the same result. However, for simplicity and to keep conformity with the previous cases, we choose u(r) = 0.

Note that, unlike the D = 1 and D = 3 cases, Eqs. (25) and (26) contain also a term with the first derivative of u. We can, however, still use the same definition of the Prüfer variables according to the ansatz (7) and (8) which, once applied to Eq. (26), generates the following first-order ODE (as for D = 3, the Prüfer variables ρ and θ refer to the case with V = 0, while for the case with $V \neq 0$ we shall use the symbols $\tilde{\rho}$ and $\tilde{\theta}$)

$$\tilde{\rho}' = \left(\frac{1}{\tilde{k}}\mathcal{V}(r)\sin[\tilde{\theta}(r)]\cos[\tilde{\theta}(r)] + \frac{m^2\sin[\tilde{\theta}(r)]\cos[\tilde{\theta}(r)]}{kr^2} + \frac{\cos^2[\tilde{\theta}(r)]}{r}\right)\tilde{\rho}(r),$$
(27)
$$\tilde{\theta}' = \tilde{k} - \frac{1}{\tilde{k}}\mathcal{V}(r)\sin^2[\tilde{\theta}(r)] - \frac{m^2\sin^2[\tilde{\theta}(r)]}{kr^2} - \frac{\sin[\tilde{\theta}(r)]\cos[\tilde{\theta}(r)]}{r},$$
(28)

with the boundary conditions $\tilde{\rho}(r) > 0$, $\tilde{\theta}(0) = 0$, and $\sin[\tilde{\theta}(L)] = 0$, with similar notation for the case with V = 0 related to Eq. (25).

$$\begin{split} \tilde{k}_{n} &= k_{n} + \frac{1}{(L-\epsilon)\tilde{k}_{n}} \int_{\epsilon}^{L} dr \mathcal{V}(r) \sin^{2}[\tilde{\theta}_{n}(r)] \\ &+ \frac{m^{2}}{(L-\epsilon)\tilde{k}_{n}} \int_{\epsilon}^{L} dr \frac{1}{r^{2}} \bigg[\sin^{2}[\tilde{\theta}_{n}(r)] - \frac{\tilde{k}_{n}}{k_{n}} \sin^{2}[\theta_{n}(r)] \bigg] \\ &+ \frac{\theta_{n}(\epsilon) - \tilde{\theta}_{n}(\epsilon)}{L-\epsilon} \\ &+ \frac{1}{(L-\epsilon)} \int_{\epsilon}^{L} dr \frac{1}{r} [\sin[\tilde{\theta}_{n}(r)] \cos[\tilde{\theta}_{n}(r)] \\ &- \sin[\theta_{n}(r)] \cos[\theta_{n}(r)]]. \end{split}$$
(29)

On choosing $\epsilon(L) = d/L^{1-\delta}$, with $1 > \delta > 0$ and *d* being constant, and by observing that the latter term of the above equation is $O(\ln(L)/L)$ which is subleading with respect to the contribution coming from the centrifugal term proportional to m^2 , which is $O(1/L^{\delta})$, we reach the same conclusions as in the case with D = 3 [14].

IV. AOC-QUANTUM-PHASE-TRANSITION ANALOGY

Our study is strictly connected to AOC. In AOC, the GS overlap of two noninteracting fermionic systems defined with the same prescriptions discussed above (i.e., two systems of N fermions confined in the same box of volume L^D , where the second system has also some potential V) decays via a power law as follows:

$$|\langle E(N,L)|\tilde{E}(N,L)\rangle|^2 \sim L^{-\gamma} = (N/\rho)^{-\gamma/D},\qquad(30)$$

where $|E(N, L)\rangle$ and $|\tilde{E}(N, L)\rangle$ are the GSs of the finite-size systems and γ is a positive exponent that depends on the phase-scattering shift. Anderson originally derived Eq. (30) in Ref. [8] by using Hadamard's inequality for the determinant and a series of steps which were clarified and set on rigorous grounds only in recent years [9,15,16]. Equation (30) implies that, in the TDL, the two GSs become orthogonal to each other, while their energies, according to Eq. (3), become equal.

It is interesting to consider the specific case of the Dirac- δ potential (see the Appendix for the case with D = 1). Either we can use the original informal bound of Ref. [8] by evaluating the phase-scattering shift from the energy shift via Fumi's theorem [17], or we can directly apply the following exact result just valid for a Dirac- δ potential [18,19] in D = 3 with strength β :

$$\gamma = \frac{\delta(\sqrt{\epsilon_F}, \beta)^2}{\pi^2},\tag{31}$$

where ϵ_F is the Fermi energy (of the system without potential) and the phase shift is given by

$$\delta(\sqrt{\epsilon_F},\beta) = \begin{cases} \tan^{-1}\left(\sqrt{\frac{\hbar^2 \epsilon_F}{2m}} \frac{1}{4\pi\beta}\right), & \beta > 0, \\ \pi - \tan^{-1}\left(\sqrt{\frac{\hbar^2 \epsilon_F}{2m}} \frac{1}{4\pi|\beta|}\right), & \beta < 0, \end{cases}$$
(32)

or, in terms of the density,

$$\delta(\sqrt{\epsilon_F}, \beta) = \begin{cases} \tan^{-1}\left(\frac{\hbar^2}{2m}\frac{\rho}{4\beta}\right), & \beta > 0, \\ \pi - \tan^{-1}\left(\frac{\hbar^2}{2m}\frac{\rho}{4|\beta|}\right), & \beta < 0. \end{cases}$$
(33)

Equation (33) shows that, as anticipated, the AOC always takes place, regardless of how β small is. But what is even more astonishing in Eq. (33) is that the phase shift is maximal in the limit of null strength; in other words, the resonance of the AOC occurs in the limit of null strength $\beta \rightarrow 0 = \beta_r$, where $\delta(\sqrt{\epsilon_F}, \beta) \rightarrow \pi/2$.

This awkward property finds an interesting counterpart within first-order quantum phase transitions (QPTs). QPTs take place, at zero temperature in the TDL, when one parameter (or more than one) of the system, let's say g, assumes a critical value g_c . At the critical point $g = g_c$, the GS energies of the two coexisting phases (the phase associated with the region $g > g_c$ and that associated with the region $g < g_c$) are equal, as prescribed by the definition of QPT of first order, while the corresponding GSs become orthogonal, as indicated by the vanishing of the associated fidelity [20]. A net example is the class of QPTs corresponding to condensation in the space of states [11], where the orthogonality of the GSs is granted by the separation of the Hilbert space in two complementary subspaces so that the scalar product in Eq. (30) vanishes (by construction it vanishes for any finite size, but only the TDL of this construction is physical [11]).

Equation (33) leads us to speculate that the resonance point $\beta_r = 0$ corresponds somehow to a critical point. In this sense, the universality of the GS energies of noninteracting systems established by Eq. (3) strongly supports this first-order QPT scenario: when the two phases "meet," they acquire the same energy and at the same time become orthogonal and resonant to each other. Interestingly, a dynamical counterpart universality was recently confirmed in the framework of heavy impurities coupled to a Fermi sea, where the AOC is enriched by the presence of an active impurity, with the impurity being part of the model with its own degree of freedom (as in the Anderson-Fano model) [21].

V. CONCLUSIONS

In the TDL, the GS energy of a system of noninteracting fermions is universal, i.e., independent of an applied potential V, provided the latter decays sufficiently fast with distance. In the case of radially symmetric potentials, we have proved that, for dimensions D = 1, 2, 3, the condition on V is actually quite mild: the integral of V(r) over the radial coordinate r may even diverge as $L^{1-\alpha}$ with any $\alpha > 0$, which means that V(r) may decay with an arbitrary small power of r.

The above result was obtained by representing the singleparticle Schrödinger equations for V = 0 and for $V \neq 0$ in terms of the Prüfer variables and looking for rigorous inequalities between the respective single-particle eigenvalues E_n and \tilde{E}_n . For a finite-size system of N fermions in a box of volume L^D , we found $\tilde{E}_n = E_n + O(1/L^{\alpha})$, with $\alpha > 0$ representing the decay power of the potential V. This result immediately provides the relation $\tilde{E}(N, L) = E(N, L) + O(\rho L^{D-\alpha})$ for the GS energies of the two systems and leads to the equality of the corresponding energies in the TDL, reached by sending N and *L* to infinity while keeping the density $\rho = N/L$ constant. Moreover, the same derivation allows us to establish that, in the case of nonpositive potentials, the number of bounded states scales as $N_0 = O(L^{D(1-\alpha/2)})$.

It is clear that the TDL equality applies not only to the GS energies but also to the energies of an equilibrium thermal state, e.g., the canonical one obtained by summing the single-particle energies E_n and \tilde{E}_n with thermal weights given by the Fermi function.

Our study is strictly connected to AOC and definitively shows that, in any AOC, the GS energies of the two systems become equal in the TDL. This result thus is in favor of an AOC-QPT analogy, where a power-law decay of the GS overlap with certain critical exponents (which may be universal or not) is a common factor. Furthermore, our analysis leads us to speculate that the resonant points of the AOC correspond somehow to the critical points of the QPT.

The analogy between AOCs and QPTs is intriguing but raises several questions. Since an AOC is definitely not a QPT, what is the physical reason for this analogy? In what sense is an AOC analogous to but different from an actual QPT? Is the limit of null strength always the resonant point in any AOC? These and other interesting issues will hopefully be the subject of future work.

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APPENDIX A: ILLUSTRATIVE EXAMPLES AND COUNTEREXAMPLES

1. One Dirac δ Confined ($\alpha = 1$)

To illustrate the universality of the GS energy, we take the straightforward example of a Dirac- δ potential in an infinite square well with D = 1. Consider a particle of mass *m* confined in the interval $x \in (-L/2, L/2)$ via hard walls and the potential

$$V(x) = -\beta \delta(x). \tag{A1}$$

The two eigenvalue problems we are interested in are then

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi(x), \quad \psi(\pm L/2) = 0,$$
(A2)

and

$$\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi(x) = \tilde{E}\psi(x), \quad \psi(\pm L/2) = 0.$$
 (A3)

The problem with V = 0, Eq. (A2), has the well-known eigenvalues

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}, \quad n = 1, 2, 3, \dots$$
 (A4)

Let us resolve the problem with $V \neq 0$. Integrating (A3) around zero gives the discontinuity of the first derivative of

the wave function

$$\psi'(0^+) - \psi'(0^-) = -\frac{2m\beta}{\hbar^2}\psi(0).$$
 (A5)

Since V is even, we can look for even and odd eigenfunctions.

Let us first focus on positive eigenvalues and let $k \in \mathbb{R}$. For the even eigenfunctions we have

$$\psi(x) = \begin{cases} A\sin(kx) + B\cos(kx), & -L/2 < x < 0, \\ -A\sin(kx) + B\cos(kx), & 0 < x < L/2, \end{cases}$$
(A6)

where A and B are suitable constants and $\tilde{E} = \hbar^2 k^2 / (2m)$. On using (A5), the boundary conditions $\psi(x = -L/2) = \psi(x = L/2) = 0$, and defining $z \equiv kL/2$, we obtain

$$\tan z = \frac{2\hbar^2}{m\beta L}z.$$
 (A7)

In the limit $L \to \infty$, Eq. (A7) has the solutions $z = n\pi$, independent of β . More precisely, for large but finite *L*, we get the energy spectrum

$$\tilde{E}_n = \frac{(2n)^2 \pi^2 \hbar^2}{2mL^2} + O\left(\frac{\hbar^4 n^2}{m^2 \beta L^3}\right), \quad n = 1, 2, 3, \dots$$
(A8)

Note that in the above expressions we assumed $\beta \neq 0$; on the other hand, if $\beta = 0$, we get exactly $z = (2n + 1)\pi/2$, and we recover the eigenenergies (A4) with an odd quantum number. For the odd eigenfunctions we have $\psi(x = 0) = 0$, so that, in this case, no discontinuity of ψ' applies, and the solutions coincide with those of the pure square-well potential:

$$\psi(x) = A\sin(kx),\tag{A9}$$

$$\tilde{E}_n = \frac{(2n)^2 \pi^2 \hbar^2}{2mL^2}, \quad n = 1, 2, 3, \dots$$
 (A10)

Let us consider now negative eigenvalues, and let $K \in \mathbb{R}$. The even eigenfunctions take the form

$$\psi(x) = \begin{cases} Ae^{Kx} + Be^{-Kx}, & -L/2 < x < 0, \\ Be^{Kx} + Ae^{-Kx}, & 0 < x < L/2, \end{cases}$$
(A11)

where *A* and *B* are suitable constants and $\tilde{E} = -\hbar^2 K^2/(2m)$. By imposing the continuity of ψ in x = 0, the boundary conditions in $x = \pm L/2$, and the discontinuity of ψ' [Eq. (A5)] and introducing $Z \equiv KL/2$, we achieve the following transcendental equation for *Z*:

$$\tanh Z = \frac{2\hbar^2 Z}{m\beta L}.$$
 (A12)

Equation (A12) admits one single nontrivial solution which exists under the condition $b \equiv (2\hbar^2)/(m\beta L) < 1$, which, in turn, is certainly satisfied for $L \to \infty$, where we get $Z \to \pm [3(1-b)]^{1/2}$ and therefore

$$\tilde{E}_0 = -\frac{6\hbar^2}{mL^2} + O\left(\frac{\hbar^4}{m^2\beta L^3}\right).$$
(A13)

Finally, concerning the odd eigenfunctions, it is easy to see that they do not exist.

Consider now N noninteracting fermions in the infinite square well. The GS energy E(N, L) is given by

$$E(N,L) = \sum_{n=1}^{N} \frac{n^2 \pi^2 \hbar^2}{2mL^2} = \frac{\pi^2 \hbar^2}{2mL^2} \left(\frac{N^3}{3} + \frac{N^2}{2} + \frac{N}{6}\right).$$
 (A14)

Similarly, in the square well including the Dirac- δ potential, by using Eqs. (A8) and (A10) as well as Eq. (A13) (which contributes as a single eigenstate, but with the lowest energy, to the GS), we obtain

$$\tilde{E}(N,L) = 2\sum_{n=1}^{N/2} \left[\frac{(2n)^2 \pi^2 \hbar^2}{2mL^2} + O\left(\frac{\hbar^4 n^2}{m^2 \beta L^3}\right) \right] + O\left(\frac{\hbar^2 N^2}{mL^2}\right) \\ = \left[\frac{8\pi^2 \hbar^2}{2mL^2} + O\left(\frac{\hbar^4}{m^2 \beta L^3}\right) \right] \\ \times \left(\frac{(N/2)^3}{3} + \frac{(N/2)^2}{2} + \frac{(N/2)}{6} \right) + O\left(\frac{\hbar^2 N^2}{mL^2}\right).$$
(A15)

On taking the ratio between (A15) and (A14), we get

$$\frac{\tilde{E}(N,L)}{E(N,L)} = \frac{8(N/2)^3}{N^3} + O\left(\frac{\hbar^2}{m\beta L}\right) + O\left(\frac{1}{N}\right).$$
(A16)

In the TDL, Eq. (A16) tends to 1, confirming the universality expressed by Eq. (3).

2. Two Dirac δ 's Confined ($\alpha = 1$)

Now, let us consider a particle in the square well with hard walls and with two Dirac- δ perturbations symmetrically located at the positions $\pm x_0$ in the D = 1 square well of length L with $L/2 > x_0 > 0$. The potential V is then

$$V(x) = -\beta\delta(x - x_0) - \beta\delta(x + x_0), \qquad (A17)$$

and the boundary conditions $\psi(-L/2) = \psi(L/2) = 0$. Let us focus on positive eigenvalues, and let $k \in \mathbb{R}$. The eigenfunctions can be written, in general, as

$$\psi(x) = \begin{cases} A_1 e^{-ikx} + B_1 e^{ikx}, & x \leqslant -x_0, \\ A_2 e^{-ikx} + B_2 e^{ikx}, & -x_0 < x < x_0, \\ A_3 e^{-ikx} + B_3 e^{ikx}, & x \geqslant x_0. \end{cases}$$
(A18)

For even eigenfunctions, the above expression takes the form

$$\psi(x) = \begin{cases} A_1 e^{-ikx} + B_1 e^{ikx}, & x \leqslant -x_0, \\ A_2 e^{-ikx} + A_2 e^{ikx}, & -x_0 < x < x_0, \\ B_1 e^{-ikx} + A_1 e^{ikx}, & x \ge x_0. \end{cases}$$
(A19)

Applying the continuity of ψ and the discontinuity of ψ' in $x = \pm x_0$, as well as the boundary conditions, we obtain the following eigenvalue equation:

$$\frac{\hbar^2}{m\beta L} = \cos^2\left(\frac{2zx_0}{L}\right)\frac{\tan z}{z} - \frac{\sin\left(\frac{2zx_0}{L}\right)\cos\left(\frac{2zx_0}{L}\right)}{z}, \quad (A20)$$

where z = kL/2. For $L \to \infty$, Eq. (A20) is reduced to

$$\frac{\tan z}{z} \to 0, \tag{A21}$$

which has a solution for $z = n\pi$. More precisely, for large but finite *L*, we get the following energy spectrum:

$$\tilde{E}_{n} = \frac{(2n)^{2}\pi^{2}\hbar^{2}}{2mL^{2}} + O\left(\frac{\hbar^{4}n^{2}}{m^{2}\beta L^{3}}\right) + O\left(\frac{2x_{0}\hbar^{2}n^{2}}{mL^{3}}\right),$$

$$n = 1, 2, 3, \dots.$$
(A22)

The odd eigenfunctions take the form

$$\psi(x) = \begin{cases} A_1 e^{-ikx} + B_1 e^{ikx}, & x \leq -x_0, \\ 2iB_2 \sin(kx), & -x_0 < x < x_0, \\ -A_1 e^{ikx} - B_1 e^{-ikx}, & x \geq x_0, \end{cases}$$
(A23)

from which we obtain the following eigenvalue equation:

$$\frac{\hbar^2 k}{2m\beta} \tan\left(\frac{kL}{2}\right) [\sin(kx_0) + \cos^2(kx_0)]$$
$$= \tan\left(\frac{kL}{2}\right) [\cos(kx_0) - \sin(kx_0)].$$
(A24)

The above equation admits the solution $\tan(\frac{kL}{2}) = 0$, i.e., $kL = 2n\pi$, n = 1, 2, 3, ..., which generates the same energy spectrum obtained at even quantum numbers for V = 0,

$$\tilde{E}_n = \frac{(2n)^2 \pi^2 \hbar^2}{2mL^2}, \quad n = 1, 2, 3, \dots$$
 (A25)

Possibly, Eq. (A24) has an extra solution for $\frac{\hbar^2 k}{2m\beta} [\sin(kx_0) + \cos^2(kx_0)] = [\cos(kx_0) - \sin(kx_0)]$; however, this solution, if any, will not be periodic and will not depend on *L*.

We skip here the analysis for negative eigenvalues since it can, at most, lead to the existence of two solutions which do not provide any net contribution to the GS in the TDL.

By using Eqs. (A22) and (A25), we can proceed analogously to the previous section and reach the following result for the ratio between the GS energies:

$$\frac{\tilde{E}(N,L)}{E(N,L)} = \frac{8(N/2)^3}{N^3} + O\left(\frac{\hbar^2}{m\beta L}\right) + O\left(\frac{x_0}{L}\right) + O\left(\frac{1}{N}\right).$$
(A26)

3. Counterexamples ($\alpha = 0$)

It is easy to exhibit counterexamples to Eq. (3); all we need is to consider a potential V whose integral scales as O(L). To stay with the case just considered of an infinite-depth square well with D = 1, assume the same boundary conditions $\psi(-L/2) = \psi(L/2) = 0$ and potential

$$V(x) = \begin{cases} V_0, & x < 0, \\ 0, & x > 0, \end{cases}$$
(A27)

with, e.g., $V_0 > 0$. A detailed calculation of the single-particle eigenvalues can be performed as in the previous sections. Here, however, we just provide simple qualitative arguments valid in the limits of large and small V_0 .

The number of eigenstates in a well of depth V_0 and width L with eigenenergies $0 < E < V_0$ is $O(\sqrt{mV_0L^2/\hbar^2})$ [13]; therefore, in the TDL with density $\rho = N/L$ being constant, we can certainly accommodate N fermions in these states provided $\sqrt{mV_0/(\hbar^2\rho^2)} \gg 1$. Moreover, if this condition is satisfied, the lowest N states can be approximated by those

of an infinite-depth well. In the present case, this means that \tilde{E}_n , for n = 1, ..., N, are approximated by Eq. (A4) with the substitution $L \to L/2$. We conclude that in the TDL $\tilde{E}(N, L)/E(N, L) \to 4$.

Conversely, if $\sqrt{mV_0/(\hbar^2 \rho^2)} \ll 1$, all eigenstates have eigenenergies $E > V_0 > 0$, so that we can estimate the effect of the potential V by standard perturbation theory. For the single-particle energies we have

$$\tilde{E}_n = E_n + \langle n|V|n \rangle = E_n + V_0/2, \qquad (A28)$$

where $|n\rangle$ are the eigenstates of the infinite-depth well and we used $\langle n|n\rangle = 1$ and $|\langle x|n\rangle|^2$ symmetric in [-L/2, L/2]. We immediately conclude that $\tilde{E}(N, L)/E(N, L) \rightarrow 1 + 3mV_0/(\pi\hbar\rho)^2$ in the TDL.

As another remarkable counterexample, consider a periodic potential. Clearly, Eq. (1) is not satisfied, so that, in agreement with Bloch's theorem, the potential V matters, and Eq. (3) does not hold.

4. A general toy model ($\alpha \ge 0$)

Above, we have shown examples where $\alpha = 1$ and counterexamples with $\alpha = 0$. In order to provide an example with

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a generic $\alpha > 0$, we should, in principle, consider a potential V(x) whose integral is weakly divergent in the TDL, for example, $V(x) = c/(|x_0|^{\alpha} + |x|^{\alpha})$. We can, however, greatly simplify this task by considering again the previous counterexample, Eq. (A27), where we now allow for a parametric dependence of V_0 on *L*:

$$V_0 = v_0 L^{-\alpha},\tag{A29}$$

where $\alpha \ge 0$ and $v_0 > 0$ are two constants. If $\alpha = 0$, we recover the previous counterexample; if instead $\alpha > 0$, for sufficiently large *L*, we have $\sqrt{mV_0/(\hbar^2\rho^2)} \ll 1$ (i.e., all eigenstates have eigenenergies $E > V_0 > 0$) and, applying Eq. (A28), we get

$$\tilde{E}_n = E_n + \langle n|V|n \rangle = E_n + \frac{v_0}{2L^{\alpha}}, \qquad (A30)$$

which leads to Eq. (2). The analysis of this toy model suggests that Eq. (1) may represent a necessary and sufficient condition for Eq. (3) to hold.

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