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On the Distribution of Eigenvalues of Grand Canonical Density Matrices

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Using physical arguments and partition theoretic methods, we demonstrate under general conditions, that the eigenvalues $w(m)$ of the grand canonical density matrix decay rapidly with their index m, like $w(m) \sim \exp[-\beta B^{-1}(\ln m)^{1+1/\alpha}]$, where B and α are positive constants, $O(1)$, which may be computed from the spectrum of the Hamiltonian. We compute values of B and α for several physical models, and confirm our theoretical predictions with numerical experiments. Our results have implications in a variety of questions, including the behaviour of fluctuations in ensembles, and the convergence of numerical density matrix renormalization group techniques.

KEY WORDS: Grand canonical ensemble; density matrix eigenvalues; partition theory; renormalization group; fluctuations.

In this Note we are concerned with the eigenvalues of the operator $\hat{\Gamma} = \exp -\beta(\hat{H} - \mu\hat{N})$. When $\hat{H}$ is the Hamiltonian, $\beta = T^{-1}$ is the inverse temperature ($k_b = 1$ for simplicity), μ is the chemical potential and N is the particle number, then this is the grand canonical density matrix operator, and its eigenvalues represent the weights of the various quantum eigenstates in the ensemble at inverse temperature β and potential μ. The eigenvalues $w(m)$ are easily determined as

$$w(m) = \exp -\beta(E_m - \mu N_m) \tag{1}$$

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where E_m and N_m are the energy and particle number of the mth eigenstate, respectively.

The rate of decay of $w(m)$ has recently generated considerable interest in the renormalization group community.[1–3] In a typical quantum lattice renormalization group study, the lattice is divided into a system and environment. One then tries to coarse-grain the system; one can do this by truncating the many-body state-space of the system to include only the important quantum states. Away from criticality, we may regard the environment as a heat bath, and consequently the system is well described by a grand canonical density matrix. If we choose to retain the first M states of the density matrix to describe the system, a measure of the truncation (coarse-graining) error is given by the weights of the states one has thrown away, i.e., $1-\sum_m^M w(m)$. The dependence of this quantity on M is in turn determined by the rate of decay of $w(m)$.

While it is clear from Eq. (1) that w decays exponentially as a function of E, a little thought shows that there can be a large number of (near) degeneracies $g(w)$ for any given value of w, which may alter the exponential decay. Thus, determining the distribution $w(m)$ first requires determining the degeneracy function $g(w)$. Partial results in this direction have previously been obtained for the Ising model by Okunishi, Hieida, and Akutsu[1] who used the theory of partitions to calculate the asymptotic behaviour of $w(m)$. However, their method directly utilised the special structure of the grand-canonical density matrix found in integrable models, such as the 1-D Ising model. They further suggest that the asymptotic form derived from the Ising model may hold universally. As we shall see, this is not quite the case, and here we generalise their approach to derive the correct form of $w(m)$ for more general classes of Hamiltonians, that encompass many physical models.

As in ref. 1, we shall rely on the theory of partitions. We present a simple generalization of the Meinardus theorem[4] from partition theory, that describes the asymptotic behaviour of the number of partitions. Although we shall only apply this result to the problem of the density matrix eigenvalues posed above, we mention in passing that many other physical problems, such as the determination of level densities in nuclei,[5] or the masses of states in string theory,[6] also admit direct partition theoretic interpretations, and our results may also be of relevance there.

We begin, however, with an "order-of-magnitude" estimate of the degeneracy $g(w)$, which illustrates in a simple way the physical ideas. Our argument is adapted from a calculation by Bethe of the degeneracy of nuclear energy levels.[7] We assume, for now, a Hamiltonian of independent particle form, i.e., $\hat{H}=\sum_i^N \hat{h}_i$. States with equal weights $w(m)=w$ have equal values of $E_m-\mu N_m$. Then, if most of the states with weight w also

have the same particle number, then they must have the same energy, and the corresponding degeneracy g is related to the entropy, through

$$g = \exp S(E). \tag{2}$$

However, we also know that the particle number distribution is strongly peaked around its equilibrium value N_0, and thus for small T, and small excitations above the ground (equilibrium ensemble) energy E_0, most excited states will have a particle number $\sim N_0$. Thus, in this simplifying case, our problem of determining $g(w)$ reduces to a calculation of the entropy. For small fluctuations we have

$$dS = \beta(dE - \mu dN). \tag{3}$$

Let us assume for simplicity that the system starts at a temperature 0, and we raise the temperature by β^{-1}. Then, the Fermi distribution function changes over a range $O(\beta^{-1})$ around the Fermi level $\mu = \epsilon_{\text{HOMO}} - \epsilon_0$, where the density of one-particle states is $O(N/\mu)$. Thus the number of excited particles is $n_e = O(N/(\mu\beta))$ (although the actual change in particle number is $dN = 0$, by our above assumption). The corresponding change in energy is

$$dE = O(\beta^{-1} n_e) = O(N/(\mu\beta^2)). \tag{4}$$

Rearranging, yields $\beta = O(N/\mu dE)^{1/2}$. Then substituting in Eq. (3), we find

$$dS = O(dE^{1/2}(N/\mu)^{1/2}). \tag{5}$$

Since the entropy at $T = 0$ is 0, $S(T) = dS$, we find approximately for the degeneracy g

$$g(dE) = \exp S \sim A \exp(BdE)^{1/2}, \tag{6}$$

where A and B are constants dependent on $\hat{H}$, and $B \propto (N/\mu)$, the density of one-particle states.

The above calculation, although crude and valid only in the regime of small fluctuations dE above the ground state, already provides an estimate of the growth of the eigenvalue degeneracy g, with increasing energy. The result is readily understood: fluctuations of $O(dE)$ are shared out across $O((BdE)^{1/2})$ single particle levels; the different combinations of these lead to the exponential dependence. Furthermore, we see that the constant in the exponential dependence is proportional to the density of one-particle states.

We should like to obtain a sharper estimate though, and this may be done through the partition theoretic approach. We recall that the number of partitions of an integer n, $g(n)$, is the number of ways that such an integer may be formed by summing positive integers less than or equal to n. If there are no further restrictions (for example, each integer may be repeated as many times in the sum as one likes), then $g(n)$ is associated with the following generating function,

$$G(q) = \sum_{n=1}^{\infty} g(n)\, q^n = \prod_{n=1}^{\infty} (1-q^n)^{-1}, \tag{7}$$

as seen by expanding in powers of q^n. Generalisations are easily constructed. For example, if some integers are to be omitted in the partition sum, the number of partitions $g(n)$ is associated with the generating function

$$G(q) = \sum_{n=1}^{\infty} g(n)\, q^n = \prod_{n=1}^{\infty} (1-q^n)^{-a_n} \tag{8}$$

where $a_n = 0$ if n is excluded, and 1 otherwise. One can obtain $g(n)$ from $G(q)$ by contour integration, using the Cauchy integral theorem, i.e.,

$$g(n) = \frac{1}{n!}\frac{d^n}{dq^n} G(q) = \frac{1}{2\pi i}\oint \frac{G(q)}{q^{n+1}}\, dq. \tag{9}$$

Remarkably, the evaluation of the above integral for certain cases of the generating function Eq. (8) may be accomplished exactly, and the history of this achievement and the mathematicians associated with it is described in ref. 8. Thus, $g(n)$ is a fairly well understood function.

In ref. 1, Okunishi *et al.* showed that the trace of $\hat{\Gamma}$ (i.e., the partition function) in the Ising model is precisely of the form Eq. (8), with $a_n = 0$ for n even. In such a case, $g(n)$ is known exactly,[8,9] and thus the eigenvalue distribution of the density matrix is also known exactly.

We are concerned, however, with more general Hamiltonians. Restricting ourselves to single particle models, let us write $f_i = \epsilon_i - \mu$, where ϵ_i is the ith eigenvalue of $\hat{h}$. Then, we have

$$w_m = \exp -\beta \sum_{j}^{N} f_j = \exp -\beta F_m. \tag{10}$$

We see that the degeneracies $g(w)$ correspond to the number of ways of forming w by summing up the eigenvalues f_i, where each f_i may only appear once (to preserve Fermi statistics). This is a generalisation of the

partition theory problem described previously, in three respects. Firstly, our eigenvalues f_i are not in general integers, secondly, there may be a bound spectrum where f_i takes negative values, and finally we have the restriction that each f_i may only appear once in any partition (i.e., all summands are distinct). It is not hard to see (described, e.g., in refs. 10, 6, and 11), that the generalization from an integer to a more general spectrum involves replacing the term q^m by q^{F_m}; furthermore restricting partitions to distinct summands is a well known problem in partition theory (see for example, ref. 8, Chap. 1), which introduces a sign change in Eq. (8), and thus the requisite generating function is

$$G(q) = \sum_{m=1}^{\infty} g(F_m)\, q^{F_m} = \prod_{m=1}^{\infty} (1+q^{f_m}). \tag{11}$$

Because of the general spectrum F_m, one cannot perform the integration in Eq. (9) exactly. However, asymptotic results applicable to Eq. (8), may be also established for our function Eq. (11). In particular, a result known as the Meinardus theorem[4, 8] (used for example, in refs. 1 and 10) yields a detailed estimate of the asymptotic $g(n)$. It is necessary to modify the theorem to encompass the three generalizations noted in the previous paragraph, but given some familiarity with the original derivation (see ref. 8, Chap. 6 for a particularly lucid exposition), the necessary corrections are not difficult to compute, and thus we state without further proof our generalised result below, valid as $F \to \infty$,

$$g(F) \sim [AF^k \exp(BF)^{\alpha/(\alpha+1)}](1+O(F^{-k'})) \tag{12}$$

where α is the real part of the rightmost (simple) pole associated with the so-called spectral zeta function $\zeta(s)$

$$\zeta(s) = \sum_{m=1}^{\infty} f_m^{-s}|_+ \tag{13}$$

and $|_+$ denotes a restriction of the above sum to positive f_m. We are interested most in the exponential form of the growth of $g(F)$, but for completeness, the constants are

$$A = 2^{\zeta(0)+n_-}[2\pi(\alpha+1)[R\Gamma(\alpha+1)\,\eta(\alpha+1)]^{\frac{1}{\alpha+1}}]^{-1/2} \tag{14}$$

$$B = (1+1/\alpha)^{1+1/\alpha}\,[R\Gamma(\alpha+1)\,\eta(\alpha+1)]^{1/\alpha} \tag{15}$$

$$k = (-1-\alpha/2)/(1+\alpha) \tag{16}$$

where n_- is the number of negative f_m in the spectrum, R is the residue of $\zeta(\alpha)$, and k' is a small number. $\eta(s)$ is the function $\eta(s) = \sum_{n=1}^{\infty} (-)^{n+1} n^{-s}$.

The above generalization differs from the original Meinardus theorem through a slightly different dependence on α and R, the presence of a different ζ function, and by the factor of $2^{\zeta(0)+n_-}$. These and other general features of the result are now discussed.

We see that the exponential growth of $g(F)$ is controlled by the position α and residue R of the rightmost (simple) pole of $\zeta(s)$. Looking back to our approximate analysis earlier, Eq. (6), we see that R is a measure of the one-particle level density, and α is a measure of its power law growth, i.e., asymptotically the eigenvalue spectrum *including the effect of degeneracies* is like $f_m \sim Rm^{1/\alpha}$. The ζ function succinctly contains all the model-specific information about the eigenvalue spectrum of the operator $\hat{h}-\mu$, and its rightmost pole describes the asymptotic behaviour of the eigenvalues. In general, the rightmost pole will lie on the positive real axis, and thus the exponent of growth in Eq. (12), $\alpha/(\alpha+1) < 1$. The determination of the exact asymptotic behaviour for a given problem, and any given Hamiltonian, thus reduces to the determination of α for the spectrum of $\hat{f}$. Since the value of α is necessarily model dependent (and varies, as we shall see, with dimensionality), it is then clear that the assertion in ref. 1, that the asymptotics of the Ising model carry over to other systems, cannot in general be true.

We note that the exponential growth of $g(F)$ is insensitive to the negative eigenvalue spectrum; in particular the ζ function is a sum restricted to only positive eigenvalues f_m. This is because for asymptotically large F, all the negative f_m are effectively 0 on the scale of F, and the states may be chosen to be occupied or unoccupied without affecting F. Thus the contribution of the negative spectrum is simply the degeneracy factor 2^{n_-}, that appears in A, Eq. (14). However, in the intermediate regime, the negative eigenvalues may lead to substantial deviations from the asymptotic form. Denoting the sum of all the negative eigenvalues f_m by $F_{\min}$, then $g(F) = \sum_{F'<0}^{F_{\min}} g_+(F+|F'|)\, g_-(F')$, where the subscripts denote partitions into positive or negative eigenvalue summands only. Then, since $g_-(F')$ is peaked at some value $|\bar{F}| = o\,|F_{\min}|$, and $\sum_{F'} g_-(F') = 2^{n_-}$, we may estimate simply by expanding the argument of the exponential,

$$g(F) \sim g_+(F)[1+O(e^{c\,|\bar{F}|\,\frac{d}{dF}F^{\alpha/(\alpha+1)}})]$$

$$\sim o(e^{c\,|F_{\min}|/F^{1/(\alpha+1)}})\, 2^{n_-} g_+(F) \tag{17}$$

Thus for $F^{1/(\alpha+1)} < |F_{\min}|$, the negative eigenvalues introduce a factor $2^{n_-} \exp c\,|F_{\min}|/F^{1/2}$ into $g(F)$.

We now illustrate our result for $g(F)$ with some explicit computations for model problems.

(i) *The d-Dimensional Harmonic Oscillator*: Consider a d-dimensional harmonic oscillator with equal fundamental frequencies in all directions, ω. The eigenvalues are then

$$\epsilon_m = \omega\left(\sum_a^d m_a + \frac{d}{2}\right), \qquad m_a = 0, 1, 2, \ldots. \tag{18}$$

The corresponding $\zeta(s)$ is the Barnes ζ function,[12, 11] which has poles at $s = d, d-1, \ldots, 1$. The residues are complicated functions of Bernoulli polynomials,[11] and we note only that they are proportional to ω^{-d}. The chemical potential μ does not affect the poles of $\zeta(s)$, and thus the rate of growth of $g(F) \sim AF^{(-1-d/2)/(1+d)} \exp(BF)^{d/(d+1)}$. Furthermore, in *any dimension*, B is proportional to ω^{-1}, which is just the one-particle eigenvalue density, as we deduced in Eq. (6).

In the case of a one-dimensional oscillator, the above expression reduces to $g(F) \sim AF^{3/4} \exp(BF)^{1/2}$. This problem is essentially isomorphic to the Ising model studied by Okunishi *et al.*,[1] and in agreement with our previous approximate result, Eq. (6). We see here the important role of dimensionality: in all dimensions, the actual one-particle eigenvalues take the same values, but because of the different degeneracies, one obtains different decays.

(ii) *Hamiltonians on a Compact Manifold*: When we restrict the Hamiltonian to act on a compact manifold, such as in a box, or the surface of a sphere, then we may use a result from the theory of elliptic differential operators, which states the poles of the corresponding $\zeta(s)$ are at (see for example refs. 13, 10, and 11) $s = (d-n)/2, n = 0, 1, 2, \ldots$, where d is the spatial dimension, with no pole at $s = 0$. (Note that this theorem does not apply to the harmonic oscillator example above, since there we do not have a compact manifold). Furthermore, the residue of the rightmost pole depends *only* on the order of the differential operator (which for most Hamiltonians is 2), the spatial dimension, and the total spatial volume.[6, 14] Thus, under the condition of compactness, the constants α and B are *universal* constants, and to leading order the asymptotic behaviour of the eigenvalue spectrum, as characterised by the function of $g(F)$, is *independent* of the detailed form of the Hamiltonian. For the relevant physical spatial dimensions, $d = 1, 2, 3$, we obtain the asymptotic forms $g(F) \sim F^{-5/6} \exp(BF)^{1/3}$, $F^{-3/4} \exp(BF)^{1/2}$, $F^{-7/10} \exp(BF)^{3/5}$, respectively.

As an example of the above type of operator, consider a particle on a d-dimensional ring (of equal radii in all dimensions, for simplicity). This

has the Hamiltonian $\hat{H} = -\Delta/2$, and corresponding eigenvalues $\sum_{a=1,d} m_a^2$, $|m| = 0, 1, \ldots$ (in suitable units); with a chemical potential, this becomes $\sum_{a=1,d} m_a^2 - \mu$. The corresponding ζ function (excluding the zeroth eigenvalue)

$$\zeta(s) = \sum_{m_a=-\infty}^{\infty} \left(\sum_{a=1,d} m_a^2 - \mu \right)^{-s} \tag{19}$$

is known as a generalised Epstein ζ function.[15, 11] This has a single first-order pole at $d/2$, with residue $R = \pi^{d/2}/\Gamma(d/2)$. This allows B to be easily calculated. For example, for $d = 2$, we find

$$g(F) \sim AF^{-3/4} \exp[2(\pi^3/6)^{1/2} F^{1/2}]. \tag{20}$$

The generality of these results may seem surprising, but it is a result of the restriction to a compact manifold. Roughly speaking, for sufficiently high eigenvalues, the spectrum of a Hamiltonian in a compact manifold begins to look like the spectrum of the Laplacian, and thus we may obtain these universal results. These results, of course, are asymptotic, and valid in the regime where $|E| \gg |V|$, where $|V|$ is the maximum of the potential on the manifold. In the intermediate regime where $|E| \sim |V|$, then other behaviour can be expected. For example, if the potential is locally quadratic, we expect the degeneracies to follow our above analysis for the harmonic oscillator.

(iii) *Coulombic Hamiltonians*: Many physical systems of interest, for example that of non-interacting electrons in the field of several nuclei, are described by Coulombic Hamiltonians. The exact treatment of such systems is not easy, and we do not have any such results to report here. Nonetheless, we can attempt to deduce some simple features of $g(F)$. The spectrum of the Hamiltonian divides into a bound and continuum region; for energies approaching 0 from below, the eigenvalues look like $-Y/n^2$, with degeneracy $2n+1$ (in 3 dimensions).

There are two new features which must thus be handled: the infinite degeneracy of the eigenvalues at $\epsilon_n = 0$ ($f_n = -\mu$, if we include the chemical potential), and the continuum nature of the positive eigenvalues. While there are techniques for handling continuum zeta functions (see for example, ref. 16), we will circumvent both these problems, since in many physical applications which concern us (for example, those that involve basis set expansion), the system of interest is studied between a minimum and maximum spatial resolution $\lambda_{\min} = 1/\kappa_{\max}$, $\lambda_{\max} = 1/\kappa_{\min}$. Under these conditions, the positive eigenvalues are like $(n\kappa_{\min})^2$, which resembles those of a particle on a ring. Furthermore, there are only a finite number of

bound eigenvalues. In the asymptotic regime with $|E| \gg |Y|$, because of the maximum spatial resolution, the analysis for compact manifolds (see above) is directly applicable, and $g(F)$ has the form shown above. As previously discussed, the bound eigenvalues lead to a degeneracy factor 2^{n-} that appears in A. Thus in 3 dimensions, we argue that the behaviour of $g(F_m)$ is as described above, viz,

$$g(F) \sim AF^{-7/10} \exp(BF)^{3/5}, \tag{21}$$

The above remarks are easily adapted to any Hamiltonian with a finite number of bound eigenvalues, and a spectrum which goes like n^β, $\beta > 0$.

(iv) *Interacting Systems*: Here, again, an exact analysis is very difficult. However, many such physical systems, even those with strong interactions, may be transformed into systems of weakly interacting pseudo-particles. For our purposes, it is sufficient to consider these as simply particles with a *fuzzy* eigenvalue spectrum, i.e., the ith energy level is $\epsilon_i + \delta\epsilon$, where $\delta\epsilon$ is a measure of the strength of interactions between pseudo-particles. Then, the results we have derived for our simple models are approximately transferable to the case of the interacting systems, where the $\zeta(s)$ function is expressed in terms of the pseudo-particle energies. (If the pseudo-particles no longer obey Fermi statistics, some modifications to the Meinardus theorem must be made, but the general features are similar).

Our results for $g(F)$, now allow us to obtain the eigenvalue distribution $w(m)$. It is clear that $m(F) = \int_{F_{\min}}^{F} g(F')\, dF'$. Since we only have an asymptotic result on $g(w)$, the integral can only be determined approximately, and we obtain

$$m(F) = O(F^{k+1} \exp(BF)^{\alpha/(\alpha+1)}). \tag{22}$$

Thus, $w(m)$ may be obtained by rearranging, (remembering $\beta F = -\ln w$), which yields

$$w(m) = O(\exp[-\beta B^{-1} (\ln m)^{1+1/\alpha}]). \tag{23}$$

This is our final result for the distribution of the eigenvalues of the density matrix, in terms of the constants A and B discussed above.

Since parts of our analysis above have been heuristic in nature, it is worthwhile to perform some numerical tests. Although our results for $\omega(m)$ are considerably cruder than those for $g(F)$, they are in the most convenient form for testing, and allow us to check the most important prediction, namely the power of the exponential growth.

Below we plot $\ln(\ln w(m))$ against $\ln(\ln m))$ for the harmonic oscillator in 1 (lines i, ii), 2 (line iii) and 3 dimensions (line iv), and for the particle

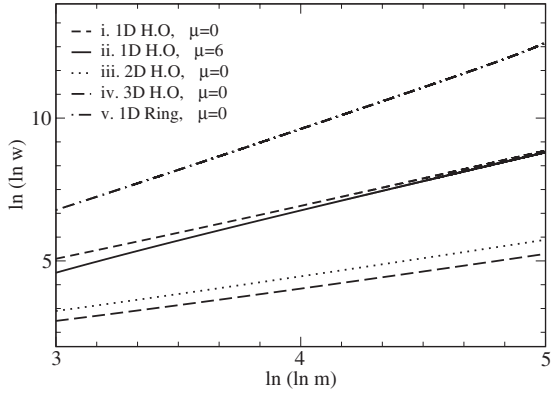

Fig. 1. Plots of $\ln(\ln w)$ against $\ln(\ln m)$, for various models.

on the ring in 1 dimension (line v). From the above result, the gradients of the lines are determined from the poles of $\zeta(s)$, as $1+1/\alpha$. Theoretically, we thus predict gradients (in the order above) of 2, 3/2, 4/3, 3, which agrees well with numerical fits to the data shown, which give 1.92, 1.26, 1.19, and 2.98. Note also how the line for the harmonic oscillator with $\mu = 6$ lies below that with $\mu = 0$, demonstrating the influence of negative eigenvalues, as described by Eq. (17).

We finish with a few comments on the utility and meaning of the results obtained. We were motivated to consider this question because of its relevance to the numerical renormalization group studies. A detailed discussion of the convergence of such algorithms is not appropriate here, but as argued in our opening paragraphs, the rapid decay of the eigenvalues indicates that the accuracy of such calculations should increase very rapidly as we keep more and more quantum states in the coarse-graining procedure. This has been suggested by previous authors.[17, 2, 3] Indeed, recent detailed numerical studies[2, 3] have demonstrated a rate of convergence in line with the theoretical prediction Eq. (23).

Finally, we mention that these results are also relevant in the more general context of fluctuations in the grand canonical ensemble. We have demonstrated that the eigenvalues of the grand canonical density matrix decay very quickly with the state index, faster than any polynomial. Thus, for any physical operator $\hat{P}$ whose expectation value $\langle P \rangle$ changes reasonably slowly with the state index m, the probability distribution of $\langle P \rangle$ in the grand canonical ensemble *is highly peaked.* For example, taking $\hat{P} = \hat{H}, N$, we see that almost all the states have the same energy and particle number, which demonstrates the well-known equivalence between the

grand-canonical and micro-canonical ensembles.[18] Note that the requirement that $\langle P \rangle$ changes reasonable slowly is analogous to the requirement that the compressibility be finite, for density fluctuations in the grand canonical ensemble to be small.

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