DEPENDENCE OF THE SPECIFIC HEAT ON THE SPECTRUM FLUCTUATIONS

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We obtain exact numerical values for the specific heat at low temperatures of a set of systems of independent fermions whose single particle energy levels follow a Poisson, Picket Fence, Uncorrelated Wigner and Gaussian Orthogonal Ensemble statistical distributions. Our results are compared with the approximate ones obtained by Denton, Mühlschlegel and Scalapino.

Consider a set of N quantum systems, each containing a fixed number $n^{(\alpha)}$ ($\alpha = 1, ..., N$) of independent fermions. The independent-particle spectrum has an average spacing δ between adjacent levels. The thermodynamic properties of the set of N quantum systems will depend on the detailed properties of their spectra, if the typical thermal energy $k_B T$ is of the order or less than δ, where k_B is Boltzmann's constant and T is the temperature. In other terms, when $\theta = k_B T/\delta \lesssim 1$, such properties as the specific heat at constant volume C_v will depend on the spacing distributions obeyed by the N spectra. This was first noted by Kubo [1], when he discussed the problem of small metallic particles at low T, which we shall mention towards the end of this note.

It is our intention here to compute C_v for sets of systems with different spectrum fluctuation properties, but all with the same δ: a set corresponding to a completely random sequence of levels, which implies a Poisson spacing distribution [2]; another one which has the same spectrum fluctuations as the Gaussian Orthogonal Ensemble of random matrices (GOE) [2]; and a set for which the spectrum consists of a Picket Fence (PF), i.e. a sequence of equally spaced levels. The corresponding nearest-neighbor spacing distributions are shown in fig. 1. Our calculation will be restricted to values of $\theta \leqslant 0.2$, since for larger values the detailed properties of the spectrum are smeared out:

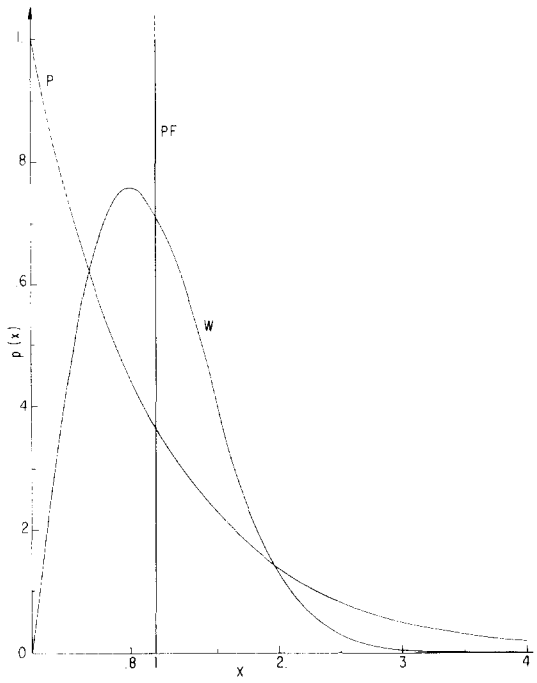

Fig. 1. Distribution of the nearest-neighbor spacings $s = E_{i+1} - E_i$, measured in terms of the average spacing δ, for the Poisson (P), Wigner (W) and Picket Fence (PF) cases. Here E_i are the single-particle energies and $x = s/\delta$.

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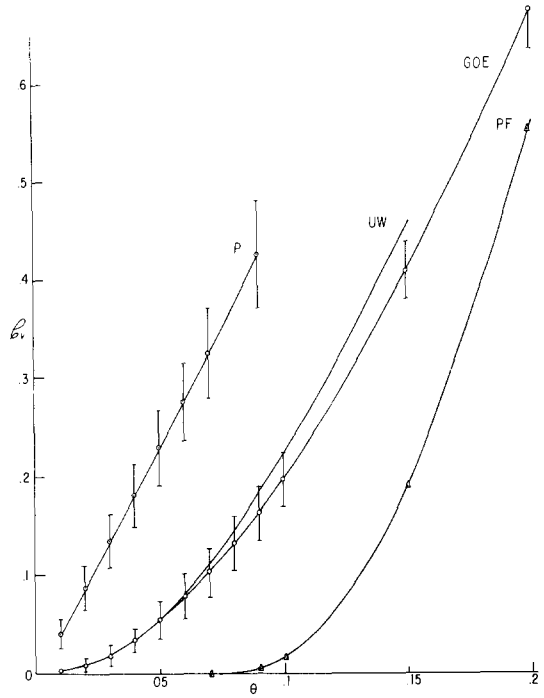

Fig. 2. Values of $\mathcal{C}_V = C_V/Nk_B$ versus $\theta = k_BT/\delta$ for a completely random spectrum (P), Uncorrelated Wigner (UW), Gaussian Orthogonal Ensemble (GOE) and equally-spaced spectrum (PF) cases. As the error bars for UW and GOE are of the same order of magnitude, only the latter are shown.

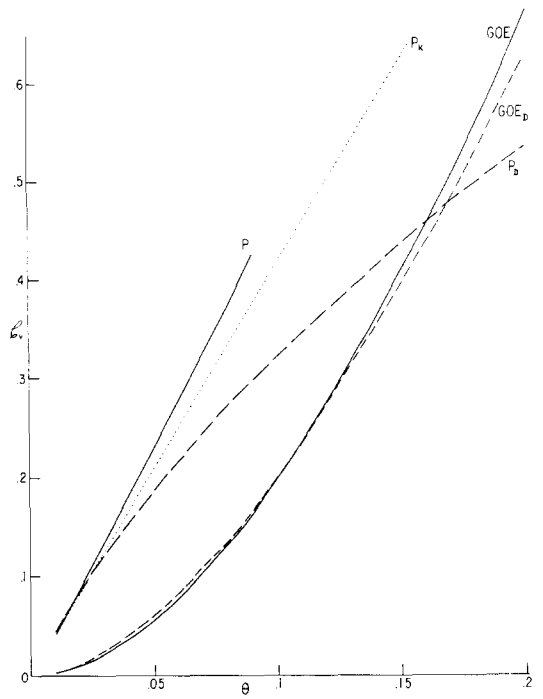

Fig. 3. Comparison of the results of this calculation (solid lines: P, GOE) with those reported in Denton et al. [5] (broken lines: P_D, GOE_D) for the specific heat $\mathcal{C}_V$ in two different cases: Poisson and GOE. Kubo's result [1] for Poisson (P_K) is also shown.

for $\theta \gtrsim 1$ all three cases lead to the same values of C_V and for $\theta \gg 1$ the spectra appear to be continuous the bulk value follows [1].

Since the number of fermions in each system is fixed, the canonical ensemble is appropriated and the specific heat $\mathcal{C}_V$ is given by [3]

$$\mathcal{C}_V = \frac{C_V}{Nk_B} = \frac{N-1}{(k_BT)^2} \sum_{\alpha=1}^{N} \frac{\{S_0^{(\alpha)}S_2^{(\alpha)} - (S_1^{(\alpha)})^2\}}{(S_0(\alpha))^2}, \qquad (1)$$

where

$$S_l^{(\alpha)} = \sum_{\lambda} g_\lambda^{(\alpha)} (\mathcal{E}_\lambda^{(\alpha)})^l \exp\{-\mathcal{E}_\lambda^{(\alpha)}/k_BT\}, \qquad (2)$$

with $l = 0, 1, 2$. Here $\mathcal{E}_\lambda^{(\alpha)}$ and $g_\lambda^{(\alpha)}$ are the energy and degeneracy of the level λ of the α-th system containing $n^{(\alpha)}$ independent fermions. As we are only interested in low values of θ, the summations can be restricted to a small number of many-fermion states for which only a few fermions are excited outside the Fermi sea; the calculation is then feasible. We therefore proceed as follows: a set of N spectra with the appropriate spacing distributions is generated by the computer and a sufficient number of single-particle states around the Fermi level are taken into account such that the S_l are obtained with a given desired precision, which in the calculation reported here is 10^{-6}.

The results of such a calculation are shown in fig. 2 for the Poisson, the GOE and the Picket-Fence cases. The values given correspond to an average over systems with even-odd number of fermions. The error bars indicated in the figure are due to the finite sampling of 2000 systems. One can see that $\mathcal{C}_V$ is largest for the first set of spectra and smallest for the equally spaced ones. This can be understood by a simple qualitative argument. At low values of θ it is the spacing between the Fermi level and the level immediately above it the only one that matters to determine $\mathcal{C}_V$. But, as is clear from fig. 1, the probability of finding a small value for this spacing is largest for the Poisson spectrum, inter-

mediate for the GOE case and smallest for the delta distribution. The ordering of the values of C_v, due to the presence of the Boltzmann factor, then follows accordingly.

We have also given in fig. 2 the results for a fourth case, labelled Uncorrelated Wigner (UW). These spectra are generated in such a way that the first nearest-neighbor spacing distribution is identical to that of the GOE case; second and higher order spacings follow the same Wigner distribution law but the spectrum is generated assuming no correlation among spacings. We can see that these correlations are not important at very low values of θ, when only the first spacing enters in the calculation, and that the value of C_v is larger for UW than for GOE when θ grows. This is so because at very low θ only one spacing matters and for both types of spectra the most probable one is, from fig. 1, $x \simeq 0.8$; for higher θ the next spacing becomes important: for UW this is uncorrelated with the previous one and, therefore, it is likely to occur also at $x \simeq 0.8$. On the other hand, for GOE the correlation coefficient between successive spacings is negative [4] and equal to 0.27, which implies that the second spacing is larger than for the UW spectrum and therefore the corresponding contribution to the Boltzmann factor will be lower in the GOE case than in the UW case.

As we mentioned before, the interest in the dependence of C_v in the spectrum fluctuations arose from the problem of the thermodynamic properties of small metallic particles at low temperatures. In this particular case, the best theoretical calculation is due to Denton et al. [5], who computed C_v assuming that only a few levels around the Fermi level follow the appropriate spectrum fluctuations, the rest being an equally spaced spectrum. It is then clear that their results will be exact for the Picket Fence case and will be better the more the spectrum resembles it. From fig. 1, we then expect their calculation to be better for the GOE than for the Poisson case. This turns out to be true, as we can see from fig. 3, where our results for C_v are compared with those of Denton et al. We also report the linear behaviour predicted by Kubo [1] in the Poisson case.

The results shown in fig. 2 are then important for the comparison with experimental values, since it is by no means clear which spacing distribution is the correct one for a powder of small metallic particles: in fact, we have given evidence [3] that random matrices do not constitute an appropriate model to represent random surface irregularities and that a Poisson spectrum might be the correct one. In any case, our fig. 2 can be considered as a morphologic chart of specific heat curves, which might be important for other quantum systems besides the powder of small metallic particles.

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