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Fourier transform of single eigenvalue probability density function using ensemble-averaged traces of the Hamiltonian

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Abstract. A determinantal identity is used to calculate the ensemble-averaged traces of the Hamiltonian. Using these averages a general expression is obtained for the Fourier transform of the single eigenvalue probability density function for all the three Gaussian ensembles for the two-dimensional case. It is shown how one can use the familiar step-up operators for the representation of a determinant. The ensemble-averaged traces are also used to derive the Fourier transform of the non-zero mean ensemble.

Keywords. Matrix ensemble theory; Fourier transform; Grassmann variables.

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1. Introduction

Since the introduction of matrix ensemble theory by Wigner (Mehta 1967), one of the challenging problems has been to study the probability density function of the single eigenvalue. The method which has been commonly followed is to transform the distribution of the Hamiltonian matrix elements to the joint distribution of the eigenvalues and eigenvector components and formally integrate over the eigenvectors to get the distribution of the eigenvalues of the Hamiltonian. Using this distribution one integrates over all the eigenvalues but one, employing special techniques, if needed, to obtain the probability density function of the single eigenvalue.

Recently (Verbaarshot *et al* 1984; Ullah 1981) it has been found to be advantageous to employ directly the Hamiltonian matrix element distribution and the invariant relations between the eigenvalues and the traces of the Hamiltonian matrix. This technique is found to be particularly useful if the ensemble is non-Gaussian. In a recent study of Gaussian unitary ensemble (Ullah 1985), it was found that the Fourier transform of the single eigenvalue probability density function has an extremely simple form. This has prompted us to study the Fourier transform of the single eigenvalue probability density function for all the three Gaussian ensembles. In the present work we shall study matrix ensembles of low dimensions only. In obtaining the Fourier transform we shall make use of the ensemble-averaged traces. The ensemble-averaged traces will be obtained using a determinantal identity in § 2. The transforms for $N = 2$ will be given in § 3. In § 4 we shall discuss the use of step-up angular momentum operators in place of Grassmann variables (Balian and Zinn-Justin 1975; Efetov 1982) in finding the ensemble average of a determinant. The technique developed in the present manuscript will also be applied to non-zero mean matrix ensembles (Edwards and Jones 1976) having $N = 2$ in §5 and the conclusion in §6.

2. Ensemble-averaged traces of the Hamiltonian

Let us consider a 2×2 Gaussian orthogonal ensemble (GOE) in which each diagonal Hamiltonian matrix element has variance $\frac{1}{2}$ and the off-diagonal element has variance $\frac{1}{4}$. We now use the well-known determinantal identity

$$\det(1 - \lambda H) = \exp\left(- \sum_{k=1}^{\infty} \frac{\lambda^k}{k} \operatorname{Tr} H^k \right), \tag{1}$$

to calculate the ensemble-averaged traces. The identity can be easily seen to be true by going over to the eigenvalues of H. Taking log, we can write the ensemble average as

$$- \sum_{k=1}^{\infty} \frac{\lambda^k}{k} \langle \operatorname{Tr} H^k \rangle = \left[\int \exp(H_{11}^2 + H_{22}^2 + 2H_{12}^2) \prod_{i \leq j} \mathrm{d}H_{ij} \right]^{-1}$$

$$\left\{ \int \ln[1 - \lambda(H_{11} + H_{22}) + \lambda^2(H_{11}H_{22} - H_{12}^2)] \right.$$

$$\left. \exp -(H_{11}^2 + H_{22}^2 + 2H_{12}^2) \prod_{i \leq j} \mathrm{d}H_{ij} \right\}. \tag{2}$$

Using first the transformation $H_{11} + H_{22} = u$, $H_{11} - H_{22} = v$ and then putting $v = \rho \cos\theta$ and $2H_{12} = \rho \sin\theta$, we get after some simplification

$$\langle \operatorname{Tr} H^k \rangle = 2^{-k} \left\{ \int_{\rho=0}^{\infty} \int_{u=-\infty}^{\infty} [\exp -\tfrac{1}{2}(u^2 + \rho^2)] \rho \mathrm{d}\rho \mathrm{d}u \right\}^{-1}$$

$$\left\{ \int_{\rho=0}^{\infty} \int_{u=-\infty}^{\infty} [\exp -\tfrac{1}{2}(u^2 - \rho^2)] [(u+\rho)^k + (u-\rho)^k] \right\}. \tag{3}$$

It is obvious from expression (3) that if k is odd then the ensemble-averaged trace vanishes. For $k = 2m$, one can carry out the integrations in (3) and obtain the following expression for $\langle \operatorname{Tr} H^{2m} \rangle$,

$$\langle \operatorname{Tr} H^{2m} \rangle = \frac{\Gamma(m + \frac{1}{2})}{\sqrt{\pi}\, 2^{m-1}} F(-m, 1; \tfrac{1}{2}; -1), \tag{4}$$

where F denotes the hypergeometric function (Abramowitz and Stegun 1965).

The same procedure can be used for the Gaussian unitary ensemble (GUE). If we again take the same variances for diagonal and the real and imaginary parts of the off-diagonal element, then we get the following expression for $\langle \operatorname{Tr} H^{2m} \rangle$,

$$\langle \operatorname{Tr} H^{2m} \rangle = \frac{\Gamma(m + \frac{1}{2})}{\sqrt{\pi}\, 2^{m-1}} F(-m, \tfrac{3}{2}; \tfrac{1}{2}; -1). \tag{5}$$

3. Fourier transform of the single eigenvalue probability density function

We first consider GUE and calculate the characteristic function $\phi(t)$ given by

$$\phi(t) = \sum_{r=0}^{\infty} \frac{(it)^r}{r!} M_r, \tag{6}$$

where M_r denotes the moments. Using expressions (5) and (6) we can write $\phi(t)$ as

$$\phi(t) = \sum_{m=0}^{\infty} \frac{1}{m!}\left(-\frac{t^2}{8}\right)^m F(-m, \tfrac{3}{2}; \tfrac{1}{2}; -1). \tag{7}$$

Using the formula which gives the sum (Hansen 1975) over hypergeometric functions, we get

$$\phi(t) = \left[\exp\left(-\frac{t^2}{4}\right)\right] M\left(-1, \frac{1}{2}, \frac{t^2}{8}\right), \tag{8}$$

where M is the confluent hypergeometric function (Abramowitz and Stegun 1965). In writing expression (8) we have also made use of Kummer's transformation (Abramowitz and Stegun 1965). Expression (8) gives the Fourier transform for the two-dimensional GUE.

We can now write the Fourier transform for all the three Gaussian ensembles by introducing parameter β which has values 1,2,4 for the GOE, GUE and Gaussian symplectic ensemble (GSE) respectively. The diagonal Hamiltonian matrix elements have now the variance $\sigma^2 = 1/\beta$ while the off-diagonal has variance $\frac{1}{2}$ of the diagonal. $\phi_\beta(t)$ is given by

$$\phi_\beta(t) = \left[\exp\left(-\frac{t^2}{2\beta}\right)\right] M\left(-\frac{\beta}{2}, \frac{1}{2}, \frac{t^2}{4\beta}\right). \tag{9}$$

We have thus shown that the Fourier transform for all the three Gaussian ensembles can be written in terms of confluent hypergeometric function.

4. Ensemble average of a determinant

The ensemble average of the log of the determinantal identify given by expression (1) becomes difficult to handle as the dimension N of the Hamiltonian matrix increases. One, therefore, takes the derivative with respect to λ and write it as

$$\sum_{k=1}^{\infty} \langle \mathrm{Tr}\, H^k \rangle \lambda^{k-1} = \left\langle \det(1-\lambda H) \frac{\partial}{\partial\lambda} \frac{1}{\det(1-\lambda H)} \right\rangle. \tag{10}$$

We then write the well-known integral representation of

$$[\det(1-\lambda H)]^{-1} = \pi^{-2} \int_{-\infty}^{\infty} \mathrm{d}x\, \mathrm{d}y\, \mathrm{d}u\, \mathrm{d}v \exp[-(x^2+u^2)(1-\lambda H_{11}) - (y^2+v^2)(1-\lambda H_{22}) + 2(xy+uv)\lambda H_{12}], \tag{11}$$

where we have taken H to be real-symmetric of dimension $N = 2$.

For the ensemble average in expression (10) one can either expand $[\det(1-\lambda H)]$ or find some suitable representation in exponential form, because we are given the distribution of the matrix elements of H as Gaussian. One such representation is through the use of anticommuting variables (Balian and Zinn-Justin 1975; Efetov 1982) of Grassman algebra. For small dimensions it turns out that one can use the familiar step-up operators l_+ for this purpose. For $N = 2$, it is easy to see that for a real-symmetric matrix A,

$$\det A = \frac{1}{24}\langle y_{22}(2)y_{22}(1)|\exp[A_{11}l_+^2(1) + A_{22}l_+^2(2) + i\sqrt{2}A_{12}l_+(1)l_+(2)]|y_{20}(2)y_{20}(1)\rangle, \tag{12}$$

where y_{lm} denote the spherical harmonics.

Assuming the distribution of H to be the one given in §2, the ensemble average indicated by expression (10) can be easily taken using expressions (11) and (12). We, therefore, write

$$\sum_{k=1}^{\infty}\langle \mathrm{Tr}\,H^k\rangle \lambda^{k-1} = \frac{1}{24\pi^2}\left(-\frac{\partial}{\partial\alpha}\right)\Big\langle y_{22}(1)y_{22}(2)\Big|$$

$$\left[\exp(l_+^2(1) + l_+^2(2) - \frac{\alpha^2}{4}l_+^2(1)l_+^2(2))\right]\int \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}u\,\mathrm{d}v \exp -(x^2+y^2+u^2+v^2)$$

$$\exp\tfrac{1}{4}[\lambda^2[(u^2+x^2)^2 + (v^2+y^2)^2 + 2(uv+xy)^2] - 2\alpha\lambda[(u^2+x^2)l_+^2(1)$$

$$+ (v^2+y^2)l_+^2(2)] - 2\sqrt{2}i\alpha\lambda[(uv+xy)l_+(1)l_+(2)]\Big|y_{20}(2)y_{20}(1)\Big\rangle_{\alpha=\lambda}. \tag{13}$$

In writing expression (13) all terms in exponential having powers of l_+ greater than two have been thrown out because they cannot connect y_{22} and y_{20}. Carrying out integrations over u, x, v, y by expressing

$$\exp\frac{\lambda^2}{4}(u^2+x^2)^2 \text{ into } \exp\frac{\lambda}{2}(u^2+x^2) \text{ etc.},$$

writing the matrix element of l_+ operators and differentiating with respect to α, and after a few simplifying steps we can write

$$\sum_{k=1}^{\infty}\langle \mathrm{Tr}\,(H^k)\rangle \lambda^{k-1} = \frac{\lambda}{2\sqrt{\pi}}\int_{-\infty}^{\infty}\mathrm{d}u\int_0^{\infty}\rho\,\mathrm{d}\rho$$

$$[1 - \sqrt{2}\lambda u + \tfrac{1}{2}\lambda^2u^2 - \tfrac{1}{2}\lambda^2\rho^2]^{-2}$$

$$[(6-\lambda^2) - 4\sqrt{2}\lambda u - \lambda^2\rho^2 + \lambda^2u^2]\exp -(u^2+\rho^2). \tag{14}$$

As earlier if k is odd, $\langle \mathrm{Tr}\,H^k\rangle$ vanishes, while if $k = 2m$, we find by carrying out integrations over u, ρ and after a few simplifying steps that

$$\langle \mathrm{Tr}\,H^{2m}\rangle = \frac{1}{\sqrt{\pi}}\frac{\Gamma(m+\frac{1}{2})}{2^{m-1}}[2mF(-m+1, 1; \tfrac{3}{2}; -1) + 1]. \tag{15}$$

Using Gauss' relations for contiguous functions it can be easily shown that

$$\langle \mathrm{Tr}\, H^{2m} \rangle = \frac{1}{\sqrt{\pi}} \frac{\Gamma(m+\frac{1}{2})}{2^{m-1}} F(-m, 1; \tfrac{1}{2}; -1), \tag{16}$$

which is precisely the same result derived earlier in § 2.

5. Non-zero mean matrix ensemble

Let us consider a 2 × 2 ensemble of real symmetric Hamiltonian in which each element has the same variance as given in § 2, but instead of zero mean, each element has a mean m. The ensemble average of the determinantal identify in this case can be written as

$$-\sum_{k=1}^{\infty} \langle \mathrm{Tr}\,(H^k) \rangle \frac{\lambda^k}{k} = \left(\int \prod_{i \leqslant j} \mathrm{d}H_{ij} \exp[(H_{11}-m)^2 + (H_{22}-m)^2 + 2(H_{12}-m)^2] \right)^{-1} \left(\int \prod_{i \leqslant j} \mathrm{d}H_{ij} \ln[1 - \lambda(H_{11}+H_{22}) + \lambda^2(H_{11}H_{22} - H_{12}^2)] \exp - \left[(H_{11}-m)^2 + (H_{22}-m)^2 + 2(H_{12}-m)^2\right] \right). \tag{17}$$

Using first the substitution $H_{11}+H_{22} = x$, $H_{11}-H_{22} = y$ and then letting $y = \rho\cos\theta$, $\sqrt{2}H_{12} = \rho\sin\theta$, $x - 2m = u$, we get

$$\langle \mathrm{Tr}\, H^k \rangle = 2^{-k} \left(\int_0^{\infty} \rho\, \mathrm{d}\rho \int_0^{2\pi} \mathrm{d}\theta \int_{-\infty}^{\infty} \mathrm{d}u \exp[-\tfrac{1}{2}(u^2+\rho^2) + 2m\rho\sin\theta] \right)^{-1} \left(\int_0^{\infty} \rho\, \mathrm{d}\rho \int_0^{2\pi} \mathrm{d}\theta \int_{-\infty}^{\infty} \mathrm{d}u [(2m+u+\rho)^k + (2m+u-\rho)^k] \exp[-\tfrac{1}{2}(u^2+\rho^2) + 2m\rho\sin\theta] \right). \tag{18}$$

Since in the present case the odd powers of $\langle \mathrm{Tr}\,(H^k) \rangle$ do not vanish, it is better to write separate expressions for even and odd k. Carrying out the integrations in expression (18), we find

$$\langle \mathrm{Tr}\, H^{2n} \rangle = \frac{\Gamma(n+\frac{1}{2})}{\sqrt{\pi}\, 2^{n-1}} \sum_{s=0}^{n} (-1)^s \frac{\Gamma(-n+s)}{\Gamma(-n)} \frac{\Gamma(\frac{1}{2})}{\Gamma(\frac{1}{2}+s)} M(-s, 1, -2m^2) M(-n+s, \tfrac{1}{2}, -2m^2), \tag{19a}$$

$$\langle \mathrm{Tr}\, H^{2n+1} \rangle = \frac{(m)}{\sqrt{\pi}} \frac{\Gamma(n+\frac{3}{2})}{2^{n-2}} \sum_{s=0}^{n} (-1)^s \frac{\Gamma(-n+s)}{\Gamma(-n)} \frac{\Gamma(\frac{1}{2})}{\Gamma(\frac{1}{2}+s)} M(-s, 1, -2m^2) M(-n+s, \tfrac{3}{2}, -2m^2), \quad n = 0, 1, 2, \ldots . \tag{19b}$$

We can now calculate the characteristic function for the non-zero mean ensemble.

Using expressions (6) and (19) and after some simplifications we can express it as

$$\phi(t) = \sum_{s=0}^{\infty} \frac{\Gamma(\frac{1}{2})}{\Gamma(\frac{1}{2}+s)}\left(-\frac{t^2}{8}\right)^s M(-s, 1, -2m^2)$$

$$\sum_{\mu=0}^{\infty} \frac{(-t^2/8)^\mu}{\mu!}[M(-\mu, \tfrac{1}{2}, -2m^2) + itm\, M(-\mu, \tfrac{3}{2}, -2m^2)]. \quad (20)$$

The sum over μ can be carried out by using the known sum formula over the Hermite polynomials (Hansen 1975) and $\phi(t)$ can finally be written as

$$\phi(t) = \exp\left(-\frac{t^2}{8} + itm\right) \sum_{s=0}^{\infty} \frac{\Gamma(\frac{1}{2})}{\Gamma(\frac{1}{2}+s)}\left(-\frac{t^2}{8}\right)^s M(-s, 1, -2m^2). \quad (21)$$

It is easy to see that if $m = 0$, $\phi(t)$ goes over to $\phi(t)$ of GOE given in §3.

6. Concluding remarks

We have shown how the Fourier transform for all the three ensembles can be obtained by calculating the ensemble-averaged traces. It is interesting to point out here that Dyson had passed a remark given in the appendix of Mehta's book (Mehta 1967) that one could derive normalization constants for all the three ensembles by replacing β by $2k$, where k is an integer, and then finding a general expression for the normalization constants valid for all k. It can be shown that if one follows the same procedure for $\phi_\beta(t)$ then the final expression is the same as the one given by expression (9) showing that the remark is valid for other quantities also.

It is shown that the determinant of a real-symmetric matrix can also be represented by using step-up operators for the two-dimensional case and one could use this representation in place of Grassman's variables to calculate ensemble averages of the determinant. It can be shown that a similar representation can also be obtained for the three-dimensional case, but beyond this one may have to use Grassman's variables only.

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