Quantum determinants: exact, approximate and numerical methods.

Studying quantum fluctuations about classical solutions we have encountered several times a problem of assembling together an infinite number of eigenvalues of a second-order differential operator,

$$\begin{aligned} \mathcal{D}\, y_n(x) &= \left[-\frac{\partial^2}{\partial x^2} + 2a(x)\frac{\partial}{\partial x} + b(x)\right]\, y_n(x) \\ &= \lambda_n\, y_n(x), \end{aligned}$$

which arises when one considers quantum fluctuations in the quadratic order.

In the case of the instanton classical solution the contribution of small quantum oscillations are assembled into

$$\frac{\text{Det}\,\mathcal{D}}{\text{Det}\,\mathcal{D}_0} = \prod_n \frac{\lambda_n}{\lambda_{0\,n}}.$$

where $\mathcal{D}_0 = -\partial^2/\partial x^2$.

In the case of the soliton solution the energy of quantum oscillations about a soliton assemble into

$$\text{Sp}\,\mathcal{D}^{1/2} - \text{Sp}\,\mathcal{D}_0^{1/2} = \sum_n \left(\lambda_n^{1/2} - \lambda_{0\,n}^{1/2}\right).$$

These objects are called functional determinants and functional traces, respectively. They are encountered in a vast number of problems in particle and condensed matter physics, and not only in relation to classical solutions.

The differential operators vary from one specific problem to another, however there are several general methods how to deal with them.

The first remark is that both objects are not far distant one from another. One writes

$$\begin{aligned} \frac{\lambda}{\lambda_0} &= \exp\left(\ln\,\lambda - \ln\,\lambda_0\right) \\ &= \exp\left(-\int_0^\infty \frac{ds}{s}\left[e^{-s\,\lambda} - e^{-s\,\lambda_0}\right]\right) \end{aligned}$$

and hence

$$\frac{\mathsf{Det}\,\mathcal{D}}{\mathsf{Det}\,\mathcal{D}_0} = \exp\left(-\int_0^\infty \frac{ds}{s}\,\mathsf{Sp}\left[e^{-s\,\mathcal{D}} - e^{-s\,\mathcal{D}_0}\right]\right).$$

Similarly,

$$\lambda^{1/2} - \lambda_0^{1/2} = \frac{1}{\Gamma(-\frac{1}{2})} \int_0^\infty \frac{ds}{s^{3/2}} \left[e^{-s\lambda} - e^{-s\lambda_0} \right], \quad \Gamma(\tfrac{1}{2}) = -2\sqrt{\pi},$$

and

$$\mathsf{Sp}\, \mathcal{D}^{1/2} - \mathsf{Sp}\, \mathcal{D}_0^{1/2} = \frac{1}{\Gamma(-\frac{1}{2})} \int_0^\infty \frac{ds}{s^{3/2}} \mathsf{Sp} \left[e^{-s\,\mathcal{D}} - e^{-s\,\mathcal{D}_0} \right].$$

In both cases one has to compute a functional trace,

$$\mathsf{Sp}\ \exp(-s\,\mathcal{D}) = \sum_n e^{-s\,\lambda_n}.$$

[Exercise: write down in a similar fashion $(\mathsf{Det}\,\mathcal{D})^{-1/2}$ and $\mathsf{Sp}(\mathcal{D}^{-1/2})$.]

How do we compute a trace of a finite-dimension operator? We first choose a complete basis, $e_m^{(\lambda)}$. For example, for a 3×3 matrix we can choose

$$e_m^{(1)} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad e_m^{(2)} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad e_m^{(3)} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

Second, we have to find the matrix elements, i.e. to sandwich the operator in question between the basis vectors, $e_m^{(\lambda)}\, M\, e_n^{(\lambda)}$. Third, we have to sum over all basis vectors, i.e. over λ and, fourth, we have to put $m = n$ and sum over m since we are computing the trace. In short,

$$\mathsf{Tr}\, M = \sum_\lambda \sum_m e_m^{(\lambda)}\, M\, e_m^{(\lambda)}.$$

[Of course, if you just see the matrix written on a piece of paper, you just sum up the diagonal elements, to get its trace. However, I needed to present this simple calculation in an abstract form, to be able to generalize it to infinite dimensions.]

Now, we have a differential operator. First, we have to choose a complete set of functions. For many cases, plane waves, e^{ipx} are sufficient. Next, we sandwich the operator in question between the plane waves which form a complete basis in the Hilbert space of functions, and sum over p:

$$\int \frac{dp}{2\pi} e^{-ipy}\, e^{-s\,\mathcal{D}}\, e^{ipx}.$$

Last, we compute the *trace*, i.e. we put $y = x$ and sum over x:

$$\mathsf{Sp}\, e^{-s\,\mathcal{D}} = \int dx \int \frac{dp}{2\pi}\, e^{-ipx}\, e^{-s\,\mathcal{D}}\, e^{ipx}.$$

We can now drag the plane wave through the exponent of the diff operator. When we succeed the exponent to the right will cancel that to the left. However,

$$\frac{\partial}{\partial x}\, e^{ipx} = e^{ipx} \cdot ip,$$

therefore the differentiation operator in $\mathcal{D}$ gets shifted by ip:

$$e^{-ipx}\, e^{-s\,\mathcal{D}}\, e^{ipx} = \exp\left(-s\,\mathcal{D}(\partial/\partial x \to \partial/\partial x + ip)\right) \cdot 1.$$

In particular, for $\mathcal{D} = -\partial^2 + 2a\,\partial + b$ the shifted operator is $-\partial^2 - 2ip\partial + p^2 + 2a\partial + 2aip + b$. Comments:

- The differentiation operator ∂ acts only on the coefficients $a(x)$, $b(x)$.
- In d dimensions one writes $\int d^d x \int d^d p/(2\pi)^d$.

- If the coefficients $a(x)$, $b(x)$ are matrices in some indices one has to take an ordinary matrix trace in those indices, on top of the functional one, $\mathrm{Tr}\exp(-s\,\mathcal{D})$.

If the 'external fields' $a(x)$, $b(x)$ are constant the functional determinant can be immediately calculated, as one can omit ∂ in the exponent:

$$
\begin{aligned}
\ln\frac{\mathrm{Det}\,\mathcal{D}}{\mathrm{Det}\,\mathcal{D}_0} &= -\int dx \int \frac{ds}{s}\int\frac{dp}{2\pi}\left[e^{-s(p^2+2iap+b)} - e^{-sp^2}\right] \\
&= -\int dx\,\frac{1}{4\sqrt{\pi}}\int\frac{ds}{s^{3/2}}\left[e^{-s(a^2+b)}-1\right] \\
&= \frac{1}{2}\int dx\,\sqrt{a^2+b}
\end{aligned}
$$

If $a(x), b(x)$ are slowly varying functions one can make a systematic expansion in the gradients, $\partial a, \partial b, \partial^2 a, \ldots$. It is called the gradient expansion. One writes

$$\exp\left[-s\left(-\partial^2 - 2ip\partial + p^2 + 2a\partial + 2aip + b\right)\right] \stackrel{d}{=} e^{A+B},$$

$$A = 2aip + b + p^2, \quad B = -\partial^2 - 2ip\partial + 2a\partial,$$

and uses the following expansion,

$$\begin{aligned} e^{A+B} &= e^A + \int_0^1 d\alpha\, e^{(1-\alpha)A}\, B\, e^{\alpha A} \\ &+ \int_0^1 d\alpha \int_0^{1-\alpha} d\beta\, e^{(1-\alpha-\beta)A}\, B\, e^{\alpha A}\, B\, e^{\beta A} + \ldots \end{aligned}$$

The differential operator B differentiates the exponents (i.e. $a(x)$, $b(x)$).

After elementary integration over α, β, p, s one gets the next terms:

$$\ln \frac{\mathrm{Det}\,\mathcal{D}}{\mathrm{Det}\,\mathcal{D}_0} = \frac{1}{2}\int dx\, \left[\left(a^2+b\right)^{1/2} + c_1 \frac{(\partial a)^2}{(a^2+b)^{3/2}} + c_2 \frac{(\partial b)^2}{(a^2+b)^{5/2}} + \ldots\right].$$

[Exercise: find the numbers $c_{1,2}$!]

The gradient expansion becomes even more powerful if the operator $\mathcal{D}$ has certain symmetry. Then the gradient expansion must be in terms of the invariants of that symmetry, e.g., gauge invariants.

Let us consider for example a scalar field interacting with the 'external'

Yang–Mills field. We shall take the case of $d = 3 + 1$. The action is

$$S = \int d^4x \, D^{ab}_\mu \phi^b \, D^{ac}_\mu \phi^c, \quad D^{ab}_\mu = \delta^{ab} \, \partial_\mu + f^{acb} \, A^c_\mu,$$

where A^c_μ are $(N^2 - 1) \cdot 4$ components of the Yang–Mills field of the $SU(N)$ gauge group.

Integrating out the scalar field $\phi^a(x)$ in a given background field $A^c_\mu(x)$ one finds the effective action of the Yang–Mills field. In fact it is a very typical problem that is encountered in numerous applications: one integrates out some quantum field (bosonic or fermionic) in a given background field, and finds the effective action of the background field. In this particular problem we have

$$e^{-S_{\rm eff}[A]} = \int D\phi^a\, e^{-S[\phi,A]} = \frac{\mathsf{Det}^{-\frac{1}{2}}(-D_\mu^2)}{\mathsf{Det}^{-\frac{1}{2}}(-\partial_\mu^2)}$$

$$= \quad \exp\left(\frac{1}{2}\int d^4x \int \frac{ds}{s}\int \frac{d^4p}{(2\pi)^4}\mathsf{Tr}\left[e^{s(D_\mu+ip_\mu)^2} - e^{-sp^2}\right]\cdot 1\right).$$

To obtain the gradient expansion of the effective action one has to expand the exponent in [...] in the covariant derivative D_μ^{ab}. Sometimes it is called the heat kernel expansion. Its $0^{\rm th}$ term is

$$\mathsf{Tr}\int \frac{d^4p}{(2\pi)^4}\, e^{-sp_\mu^2} = (N^2-1)\,\frac{1}{16\pi^2\, s^2}$$

but it cancels with the subtracted term corresponding to ‘free’ (no external field) determinant. The linear term, $isp_\mu D_\mu$ is zero (as are all odd terms) because of integration over p_μ. The quadratic term in D_μ comes from two sources,

$$\begin{aligned} & \mathsf{Tr} \int \frac{d^4p}{(2\pi)^4} \, e^{-p^2 s} \left[D^2 s + \frac{1}{2!} (2i)^2 s^2 \, D_\alpha D_\beta \, p_\alpha p_\beta \right] \\ = \quad & \mathsf{Tr} \, \frac{1}{16\pi^2} \left(D^2 \frac{1}{s} - D^2 \frac{1}{s} \right) = 0, \end{aligned}$$

which is nice since $D^2 \cdot 1 \sim A_\mu^2$ is not gauge invariant. Such term cannot be present in the effective action which must be gauge-invariant!

The quartic term is

$$\frac{1}{6 \cdot 16\pi^2} \, \mathsf{Tr}(D_\alpha D_\beta D_\alpha D_\beta - D_\alpha D^2 D_\alpha)$$

$$= \frac{1}{12\cdot 16\pi^2}\,\mathsf{Tr}[D_\alpha D_\beta][D_\alpha D_\beta] = -\frac{N}{12\cdot 16\pi^2}\,F^a_{\alpha\beta}F^a_{\alpha\beta},$$

where we have used

$$[D_\alpha D_\beta] = f^{acb}\,F^c_{\alpha\beta}, \quad f^{abc}\,f^{abd} = N\,\delta^{cd}.$$

This is the lowest order gauge invariant, coinciding, as a matter of fact, with the Yang–Mills action.

To get the $6^{\rm th}$-order term one has to work for a while. The result is expressed through two new gauge invariants,

$$\frac{N}{16\pi^2}\,s\,\left(\frac{1}{60}(D^{ab}_\alpha F^b_{\alpha\gamma})(D^{ac}_\beta F^c_{\beta\gamma}) - \frac{1}{180}\,f^{abc}\,F^a_{\alpha\beta}\,F^b_{\beta\gamma}\,F^c_{\gamma\alpha}\right)$$

Combining the results we get the expansion in terms of gauge invariants:

$$\text{Sp}\left[e^{sD^2} - e^{s\partial^2}\right] = \frac{N}{16\pi^2}\left[-\frac{F_2}{12} + s\left(\frac{I_3}{60} - \frac{F_3}{180}\right) + O(s^2)\right],$$

$$F_2 = \int d^4x\, F^a_{\alpha\beta}F^a_{\alpha\beta}, \ldots$$

This must be now integrated over $\int ds/s$ and we see that the first term of the heat kernel expansion leads to a logarithmic divergency. It is to be expected: scalar field loops lead to a renormalization of the gauge coupling constant $1/g^2(\mu)$ standing in front of the YM action F_2, and we are about to calculate this renormalization.

One can use different regularization methods to tame the logarithmic divergency. One example is Pauli–Villars regularization: consider the ‘quadrupole formula’

$$\frac{\text{Det}^{-\frac{1}{2}}(-D^2)}{\text{Det}^{-\frac{1}{2}}(-\partial^2)}\frac{\text{Det}^{-\frac{1}{2}}(-\partial^2+\mu^2)}{\text{Det}^{-\frac{1}{2}}(-D^2+\mu^2)} \to \times\left(1-e^{-\mu^2\, s}\right)$$

A more simple way is just to cut the s integration from below by some $s_0 = 1/\mu^2$. The variable s is called proper time, and this is called proper-time regularization. In any case we find that scalar fields renormalize the gauge coupling by

$$\frac{1}{g^2(\mu)} - \frac{N}{48\pi^2}\ln\frac{\mu}{\Lambda}.$$

There exists a naive method which, however, allows to evaluate functional determinants quickly and with a rather good accuracy in situations where exact calculations are hopeless and numerical calculations are time-consuming. see D.D., V. Petrov and A. Yung, *Phys. Lett.* B130 (1983) 385

Generically, one has to calculate

$$\frac{\mathrm{Det}\,\mathcal{D}}{\mathrm{Det}\,\mathcal{D}_0} = \exp\left(-\int_0^\infty \frac{ds}{s}\,\mathrm{Sp}\left[e^{-s\,\mathcal{D}} - e^{-s\,\mathcal{D}_0}\right]\right).$$

We write

$$\int_0^\infty ds \ldots = \int_0^\delta ds \ldots + \int_\delta^\infty ds \ldots$$

In the first integral we assume that δ is small enough so that one can replace Sp[...] by a few terms of the derivative expansion. In the second integral one assumes that δ is large enough so that Sp[...] can be replaced by a few lowest eigenvalues, $\sum e^{-s\lambda_n}$. Both actions are approximate, however, varying the sum of two integrals in δ and finding δ from the requirement that the variation to zero one may hope to minimize the error.

Let us show how it works in the example of Det$(-D_\mu^2)$. The operator is positive-definite and has no zero modes. Therefore, we just neglect the second integral. The first integral,

$$\int_0^\delta \frac{ds}{s}\left[-\frac{F_2}{12}+s\left(\frac{I_3}{60}-\frac{F_3}{180}\right)\right],$$

has an extremum in δ at

$$\delta=\frac{15F_2}{3I_3-F_3}$$

Substituting this value back into the integral's upper limit we get

$$\left(\frac{\mathsf{Det}^{-\frac{1}{2}}(-D^2)}{\mathsf{Det}^{-\frac{1}{2}}(-\partial^2)}\right)_{\mathrm{reg}} \approx \exp\left(-\frac{N\,F_2}{24\cdot 16\pi^2}\,\ln\mu^2\,\delta\right).$$

There is an example where this determinant has been computed exactly: it is the case of the Yang–Mills instanton. For the instanton background field

$$\begin{aligned} F_2 &= 32\pi^2, \quad F_3 = -\frac{12}{5}\,32\pi^2\,\frac{1}{\rho^2}, \quad I_3 = 0, \\ \delta &= \frac{25}{4}\,\rho^2 \end{aligned}$$

where ρ is the instanton size. We obtain

$$\left(\frac{\text{Det}^{-\frac{1}{2}}(-D^2)}{\text{Det}^{-\frac{1}{2}}(-\partial^2)} \right)_{\text{reg}} \approx (\mu\rho)^{-N/6}\, e^{-N\cdot 0.153}$$

which should be compared with the exact result obtained by G. 't Hooft, *Phys. Rev.* D14 (1976) 3432:

$$(\mu\rho)^{-N/6}\, 1.073 \cdot\, e^{-N\cdot 0.190}.$$

A more clever approximate method of evaluating Det's will be considered later.

There are two ways how a functional determinant in a background field can be found exactly.

1) For some specific external fields the analogous Schrödinger eqn, $\mathcal{D}y_n = \lambda_n y_n$, is for more or less accidental reasons exactly solvable, so that one find exactly all eigenvalues λ_n; their product is the functional determinant. Lucky examples:

a. Quantum fluctuations about a kink in $1d$.
b. Quantum fluctuations about $CP(N-1)$ instantons in $2d$.
c. Quantum fluctuations about Yang–Mills instantons in $4d$.

2) Functional determinants in certain generic backgrounds are exactly computable when they are fully determined by quantum anomalies, next lecture.

In many cases the functional form of the oscillation determinants can be found from symmetry considerations, up to a overall factor of the order of unity. This factor can be either estimated using the DPY method (see above) or computed numerically.

Numerical methods

For a given background field, the functional determinant (or the sum of eigenvalues, in case of the soliton) can be found numerically as follows.

1) One chooses a complete set of functions which can serve as a basis. In $1d$ these can be plane waves, e^{ipx}, in $2d$, if there is an axial symmetry in the problem, one can choose $e^{im\phi}\,J_m(k\rho)$, in $3d$ with spherical symmetry spherical harmonics $Y_{l\,m}(\theta,\phi)\,j_l(kr)$ can do the job.

2) Apart from a few zero modes, the differential operator has a continuous spectrum; to deal with it numerically one needs to discretize the spectrum by putting the system in a box and require that the basis wave functions

are zero at the boundaries. It gives a discrete spectrum:

$$
\begin{aligned}
d = 1: \quad p_n &= \frac{2\pi n}{L}, \quad L = \text{box length}, \\
d = 2: \quad k_n &= \frac{z_{mn}}{R}, \quad R = \text{box radius}, \\
z_{mn} &= \text{n}^{\text{th}} \text{ zero of } J_m(z), \\
d = 3: \quad k_n &= \frac{z_{ln}}{R}, \quad R = \text{box radius}, \\
z_{ln} &= \text{n}^{\text{th}} \text{ zero of } j_l(z).
\end{aligned}
$$

The size of the box should be taken $>>$ than the typical spatial size of the background field. Eventually, one has to verify that the results do not depend on R.

3) One also has to regularize the determinant, for example by restricting

momenta by some $k_n < k_{\max}$. If the determinant is finite one has to check that the result does not depend on $k_{\max}$; if one expects renormalization, the (known) dependence of the result on $k_{\max}$ can be used to check the numerics.

4) One sandwiches the operator in question between the chosen basis functions and computes the matrix elements,

$$\mathcal{D}_{MN} = \int d^d x \, f^\dagger_M(x) \, \mathcal{D} \, f_N(x).$$

With regularization and discretization, it is a finite-dimension matrix (say, 100×100); one find its eigenvalues numerically.

5) The product of the eigenvalues is the determinant.
See, e.g. D.D. et al., *Phys. Rev.* D49 (1994) 6864
A *Mathematica* Program for Computing Heat Kernel Coefficients:

M. Booth, hep-th/9803113 v3