Physics 210- Fall 2018

Classical and Statistical mechancis

Solution to Home Work # 1
Solution posted 31 October 2018

1. *Functional derivatives*
Consider a functional of a function $\Psi(x)$

$$F[\Psi] = \int_0^L dx\{\frac{a}{2}|\Psi'(x)|^2 + \frac{1}{2}|\Psi(x)|^2 + \frac{g}{4}|\Psi(x)|^4\}.$$

a) Assuming Ψ is a real function calculate the functional derivative $\frac{\delta F}{\delta \Psi(x)}$. . . . [5]

Let me first indicate how I calculate the functional derivatives, this is equivalent to other methods but I find it convenient. I will set $\Psi(x) \to \Psi(x) + \delta\Psi(x)$, then *linearize* in $\delta\Psi(x)$ to write

$$F[\Psi + \delta\Psi] - F[\Psi] = \int_0^L dx\, \delta\Psi(x)\, \frac{\delta F}{\delta \Psi(x)} + O((\delta\Psi)^2),$$

and thereby read off the functional derivative $\frac{\delta F}{\delta \Psi(x)}$. Calculating the right hand side (RHS) and throwing out terms of $O(\delta\Psi)^2$, we get

$$RHS = \int_0^L dx\, \delta\Psi(x)\, \left(\Psi(x) + g\Psi^3(x) - a\Psi_{xx}(x)\right) + a\left[\delta\Psi(x)\Psi_x(x)\right]_0^L.$$

I am using $\Psi_x(x) = \Psi'(x) = \frac{d}{dx}\Psi(x)$, and similarly $\Psi_{xx}(x)$ for the second derivative. The boundary term is obtained by the usual rules of integration by parts, and reads as

$$[\delta\Psi(x)\Psi_x(x)]_0^L = \delta\Psi(L)\Psi_x(L) - \delta\Psi(0)\Psi_x(0).$$

This term needs to be understood properly. Usually we ignore the boundary terms, assuming implicitly that something will kill them, e.g. boundary conditions. We will see the role of these below, but in general it is good to keep in mind that the boundary terms can be non-zero. First let us kill the boundary terms, in which case

$$\frac{\delta F}{\delta \Psi(x)} = \Psi(x) + g\Psi^3(x) - a\Psi_{xx}(x).$$

Next think of an example where nothing else is given about the boundary terms. In such a case we may deduce that

$$\frac{\delta F}{\delta \Psi(x)} = \Psi(x) + g\Psi^3(x) - a\Psi_{xx}(x) + 2a(\delta(x-L) - \delta(x))\Psi_x(x),$$

where I have added a factor of 2 multiplying a in the boundary term, to accomodate the usual definition

$$\int_0^a dx\, \delta(x) = \frac{1}{2}.$$

You can plug this into the integral and verify that we reproduce the RHS. In such a case the functional derivative picks up two boundary delta functions.

b) Assuming Ψ is a complex function calculate the functional derivative $\frac{\delta F}{\delta \Psi^*(x)}$. Here you may assume Ψ, Ψ^* are independent of each other. ... [5]

It is important to note that we can vary both Ψ and Ψ^* *independently* for the complex Ψ, whereas if Ψ is taken as real then we have modify this and only vary $\Psi \to \Psi + \delta\Psi$. In classical mechanics we rarely come across the complex case, but in quantum theory it is very common since the wave functions are allowed to be complex. I will set $\Psi(x) \to \Psi(x), \Psi^*(x) \to \Psi^*(x) + \delta\Psi^*(x)$, then *linearize* in $\delta\Psi^*(x)$ to write

$$F[\Psi^* + \delta\Psi^*, \Psi] - F[\Psi^*, \Psi] = \int_0^L dx\, \delta\Psi^*(x)\, \frac{\delta F}{\delta \Psi^*(x)} + O((\delta\Psi^*)^2),$$

and thereby read off the functional derivative $\frac{\delta F}{\delta \Psi^*(x)}$. Notice that i wrote $F \equiv F[\Psi^*, \Psi]$ to emphasize the equal footing of Ψ and Ψ^*.

Hence carrying through the above

$$RHS = \int_0^L dx \delta\Psi^*(x) \frac{1}{2}\left(\Psi(x) + g\Psi^3(x) - a\Psi_{xx}(x)\right),$$

assumed conditions such that the boundary term is thrown out. Note the extra factor $\frac{1}{2}$ here relative to the case of real Ψ, it arises from the fact that while varying Ψ^* the Ψ is unchanged and hence does not contribute to the integrals.

c) In the first case compare the fixed boundary condition (i) $\delta\Psi(0) = 0 = \delta\Psi(L)$ and the periodic boundary condition (ii)$\delta\Psi(0) = \delta\Psi(L) \neq 0$ together with $\Psi'(0) = \Psi'(L)$. ...[5]

Note that the boundary term

$$\delta\Psi(L)\Psi_x(L) - \delta\Psi(0)\Psi_x(0)$$

vanishes in both cases. One may say that the conditions are tailored that this happens.

d) Assuming case (a) and periodic boundary conditions, find the function $\Psi(x)$ which minimizes the functional F at $g = 0, a = 1$ under the constraint of fixed magnitude $\int_0^L dx\Psi(x)|^2 = 1$. (Here you need to set up a differential equation for Ψ and solve it in the case when $g = 0$. This is easy since $g = 0$ reduces it to a linear differential equation.) ...[5]

Let us set up a Lagrange multiplier scheme

$$\hat{F} = F + \lambda\left(\int_0^L dx\, \Psi^2(x) - 1\right)$$

so that if the constraint of normalization is satisfied then the second term drops out and we are minimizing the old functional F. Taking the functional derivative and putting it to zero we get the minimizing function from

$$-\Psi_{xx} + \Psi(x) + 2\lambda\Psi(x) = 0.$$

We can solve this differential equation easily and find the solutions

$$\Psi(x) = \alpha e^{\pm x\sqrt{1+2\lambda}},$$

where α is a normalization constant, which can be determined along with λ shortly hereafter. In order to satisfy periodic boundary conditions this solution implies

$$1 = e^{\pm L\sqrt{1+2\lambda}},$$

which has only one sensible solution if we choose

$$\lambda = -\frac{1}{2},$$

and hence the solution for Ψ reads

$$\Psi(x) = \frac{1}{\sqrt{L}},$$

together with the value for $\lambda = -\frac{1}{2}$. Let us now plug this into the functional F, or $\hat{F}$ (it makes no difference as we showed above), thus

$$F_{min} = \frac{1}{2}.$$

To show that there is a minimum for F is also possible- we may take the second functional derivative and show it is positive.

2. *Differential equations and difference equations. Use any convenient software for help with this problem, e.g. Mathematica, Matlab,..*

   Consider the 1-d anharmonic oscillator in dimensionless form

$$H = \frac{p^2}{2} - \frac{x^2}{2} + \frac{x^4}{4}.$$

   a) Write the Lagrangian and Hamiltonian equations of motion. ...[5]

   We may write Hamilton's EOM

$$\dot{x} = \frac{\partial H}{\partial p} = p$$
$$\dot{p} = -\frac{\partial H}{\partial x} = x - x^3$$

   To find the Lagrangian we carry out

$$L = \dot{x}p - H = \frac{\dot{x}^2}{2} + \frac{x^2}{2} - \frac{x^4}{4}$$

   The Lagrange EOM are

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}} - \frac{\partial L}{\partial x} = 0$$
$$\ddot{x} - x + x^3 = 0$$

   b) Using the discretization $t = j\Delta t,\ j = 0, M-1$, with a variable M, convert these two equations to difference equations. Solve the two sets of equations from t=0 to t= 10, by iteration for M=10,100,1000 with initial conditions $x(0) = 0; q(0) = \dot{x}(0) = 0.2$ and compare the various solutions. ...[5]

   Numerics

   c) Using a representative M, compare the Hamilton equations solutions with the case $x(0) = -1, q(0) = \dot{x}(0) = 0.2$. ...[5]

Numerics

d) Draw the phase portraits of the oscillator, by eliminating t and plotting p versus x by exploring various values of the energy of the oscillator. We expect to see circles surrounding the two points $x = \pm 1$ representing small oscillations around the equilibrium, and a larger set of closed curves surrounding both. These would be separated by a "critical curve" called the separatrix. (This problem has a large fan following in the internet so you should be able to get some help using google scholar.) ...[5]

Numerics

3. *Poisson brackets:*

Writing briefly $[] \equiv []_{PB}$, show the properties

a) For any three functions

$$\begin{aligned} [f,g] &= -[g,f] \\ [f+g,h] &= [f,h]+[g,h] \\ [fg,h] &= f[g,h]+[f,h]g \\ [f,[g,h]]+[g,[h,f]]+[h,[f,g]] &= 0, \text{ Jacobi's identity} \end{aligned}$$

...[5]

Standard exercise

b) Calculate the PB's $[q_i, p_j^3]$, $[Exp[3q_i], p_j^2]$ ...[5]

$$[q_i, p_j^3] = \frac{\partial p_j^3}{\partial p_i} = 3p_i^2 \delta_{ij}.$$

$$[Exp[3q_i], p_j^2] = \frac{\partial Exp[3q_i]}{\partial q_i} \frac{\partial p_j^2}{\partial p_i} = 6Exp[3q_i]\; p_i\; \delta_{ij}.$$

4. *Legendre Transforms: General theory and examples*

We may define the Legendre Transform (LT) of any function $F(x)$ as

$$G(y) = \{yx - F(x)\}_{LT} = yx(y) - F(x(y)) \tag{1}$$

where

$$F'(x(y)) = y,$$

i.e. at a given y, we solve for $x(y)$ where the slope of F matches y.

An often added convention: If multiple solutions of $F'(x) = y$ exist, the convention is to choose the solution for which $G''(y) > 0$ i.e. G is a concave-up function of y.

Note: In Eq. (1) we have chosen the sign using the CM convention (used in Classical Mechanics). In Thermodynamics and Stat Mech we will use the SM convention (i.e. the opposite convention), multiply the RHS by -1. With the CM convention the LT of a concave-up function is another concave-up function, while with the SM convention the LT of a concave-up function is another concave-down (or equivalently convex up) function.

a) Calculate $G(y)$ the LT of

$$F(x) = e^{x-1}.$$

. . . [5]

b) Calculate the LT of $G(y)$ and show that we get back $F(x)$. . . . [5]

c) Calculate the LT of

$$F(x) = \frac{x^2}{2} - \frac{x^3}{3}.$$

Show that this leads to two functions $G_1(y)$ and $G_2(y)$. Show that only one of these satisfies the concave-up convention. Graph these functions over a sensible region of x, y . . . [5]

d) Calculate the LT of G_1 and G_2 found above, and show that only one of them recovers the $F(x)$. . . . [5]

See Mathematica notebook on the Course website, and pdf and also CDF file of solution. It includes a simple package for LT of any function

5. Considering a relativistic Hamiltonian (1-d)

$$H = \sqrt{p^2c^2 + m^2c^4} + U(q),$$

a) Find Hamilton's equations of motion. . . . [5]

$$\begin{aligned} \dot{q} &= \frac{\partial H}{\partial p} = \frac{pc^2}{\sqrt{p^2c^2 + m^2c^4}} \\ \dot{p} &= -\frac{\partial U(q)}{\partial q} \end{aligned}$$

b) Carry out the LT to calculate the Lagrangian. Comment on the form of the kinetic energy in the Lagrangian- is the result what one might have expected? ... [5]

$$L(\dot{q}, q) = \dot{q}p - H(p, q)$$

We need to solve for p in terms of the velocity and plug in. From Hamilton's EOM inverting the first equation we get

$$p = \frac{m\dot{q}}{\sqrt{1 - \frac{\dot{q}^2}{c^2}}}$$

where we discarded a possible solution with a negative sign for physical reasons (think of $c \to \infty$ limit). Plugging in we get after a brief calculation

$$L = -mc^2\sqrt{1 - \frac{\dot{q}^2}{c^2}} - U(q).$$

If we expand in the limit of large c, the leading term gives us the usual non-relativistic Lagrangian $\frac{m}{2}\dot{q}^2 - U(q)$, apart from a constant.

c) From the Lagrangian calculate the Lagrange equations of motion, and show that they are the same as those in (a). ... [5]

Easy

6. To describe the electromagnetic field interacting with a charged particle in 3-d,we use a Lagrangian

$$L = \frac{m}{2}\dot{\vec{r}}.\dot{\vec{r}} - q_e(\Phi(r) - \frac{1}{c}\dot{\vec{r}}.\vec{A}(\vec{r})) - V(\vec{r}),$$

where q_e is the electron charge, the vector potential $\vec{A}$ and scalar potential Φ lead to EM fields through the usual relations

$$\vec{\nabla} \times \vec{A}(r) = \vec{B}(r),$$

$$\vec{E} = -\vec{\nabla}\Phi(r) - \frac{1}{c}\frac{\partial \vec{A}}{\partial t},$$

and $V(\vec{r})$ is an arbitrary external potential.

a) Using the Legendre transforms, find the Hamiltonian for this problem. ... [5]

From $p = \partial L/\partial \dot{q}$ we deduce

$$\dot{\vec{r}} = \frac{1}{m}\left(\vec{p} - \frac{q_e}{c}\vec{A}\right).$$

The term $m\dot{\vec{r}}$ is often called the kinetic momentum, which differs from the "canonical momentum" p by the second term. Substituting we get

$$H = \vec{p}.\dot{\vec{r}} - L = \frac{1}{2m}\left(\vec{p} - \frac{q_e}{c}\vec{A}\right)^2 + q_e\Phi + V(\vec{r})$$

b) While L is linear in $\vec{A}$, note that H is quadratic in A. Do you think this quadratic dependence can have observable effects? (A brief answer will suffice). . . . [5]

This question has a different answer in classical mechanics and in quantum mechanics. In classical mechanics, the vector potential does not change the energy since it can do no work. There is a famous theorem of Miss van Leeuwen and Niels Bohr in Stat Mech to this effect. In quantum theory the quadratic dependence leads to the important phenomenon of *diamagnetism*, which is relevant in systems as diverse as superconductors (Meissner effect says all fields are expelled from a superconductor) to various fluids studied in physics/chemistry.

c) From the Lagrange equations of motion show that the force experienced by a particle is

$$m\ddot{\vec{r}} = -\vec{\nabla}V + q_e\{\vec{E} + \frac{\dot{\vec{r}} \times \vec{B}}{c}\}.$$

Note that the second term is the familiar Lorentz force, it is this equation that justifies the choice of the Lagrangian. . . . [10]

It is helpful to use cartesian indices and the repeated symbol summation convention of Einstein to deal with the vectors here. Let us write the fields in index form

$$E_j = -\partial_j\Phi - \frac{1}{c}A_j, \quad B_i = \varepsilon_{ijk}\partial_j A_k.$$

Now Lagrange's EOM says

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{r}_j} = \frac{\partial L}{\partial r_j}.$$

Let us work out a few items

$$\begin{aligned}\frac{\partial L}{\partial \dot{r}_j} &= m\dot{r}_j + \frac{q_e}{c}A_j \\ \frac{\partial L}{\partial r_j} &= -\partial_j V - q_e\partial_j\Phi + \frac{q_e}{c}\dot{r}_i\partial_j A_i\end{aligned}$$

Note that in the last equation, the repeated index i (rather than j an external index) which is summed over. In taking the time derivative $\frac{d}{dt}$ we should keep track of the fact that it is a total derivative.

Thus

$$\frac{d}{dt}f(r,t) = \frac{\partial f(r,t)}{\partial t} + \dot{r}_j\frac{\partial f(r,t)}{\partial r_j},$$

and hence

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{r}_j} = m\ddot{r}_j + \frac{q_e}{c}\frac{\partial A_j}{\partial t} + \frac{q_e}{c}\dot{r}_k\frac{\partial A_j}{\partial r_k}.$$

Plugging into the EOM we find

$$m\ddot{r}_j = -\partial_j V - q_e\partial_j\Phi - \frac{q_e}{c}\frac{\partial A_j}{\partial t} + \frac{q_e}{c}\left(\dot{r}_k\partial_j A_k - \dot{r}_k\partial_k A_j\right).$$

Combining terms to form the fields we write this as

$$m\ddot{r}_j = -\partial_j V + q_e\left(\vec{E} + \frac{1}{c}\dot{\vec{r}}\times\vec{B}\right)_j. \quad \text{(QED)}$$

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