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[disclaimer]

physics606 – Advanced Quantum Theory

Problem Set 3

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problem number	achieved points	possible points
1		14
2		9
3		10
Total		33

1 Particle in external electromagnetic field

1.1 Canonical momentum

In general, the canonical momenta in classical mechanics are defined as

$$\pi_i := \frac{\partial L}{\partial \dot{x}^i}.$$

We use $\boldsymbol{\pi}$ instead of $\boldsymbol{P}$ here to make the distinction to the linear momentum $\boldsymbol{p}$ clearer.

Given the particular Lagrange function we have:

$$\pi_i = m\dot{x}_i + qA_i.$$

The linear momenta are given by

$$p_i = m\dot{x}_i$$

and differ by the qA_i in the canonical momenta.

1.2 Hamilton function

Generally, the Hamilton function is defined as

$$H(q,\pi,t) := \pi_i \dot{q}^i(q,\pi,t) - L(q,\dot{q}(q,\pi,t),t).$$

The velocities all have to be replaced with the canonical momenta. The velocities are given by

$$\dot{x}_i = \frac{1}{m}[\pi_i - qA_i]$$

which need to be inserted into the Hamilton function.

The Hamilton function is

$$\begin{aligned}
H &= \pi_i \dot{q}^i - L \\
&= \boldsymbol{\pi}\dot{\boldsymbol{x}} - \frac{m}{2}\dot{\boldsymbol{x}}^2 + qU - q\dot{\boldsymbol{x}}\boldsymbol{A} \\
&= \frac{1}{m}\boldsymbol{\pi}[\boldsymbol{\pi} - q\boldsymbol{A}] - \frac{1}{2m}[\boldsymbol{\pi} - q\boldsymbol{A}]^2 + qU - \frac{q}{m}[\boldsymbol{\pi} - q\boldsymbol{A}]\boldsymbol{A} \\
&= \frac{1}{m}[\boldsymbol{\pi} - q\boldsymbol{A}]\left[\boldsymbol{\pi} - \frac{1}{2}[\boldsymbol{\pi} - q\boldsymbol{A}] - q\boldsymbol{A}\right] + qU \\
&= \frac{1}{m}[\boldsymbol{\pi} - q\boldsymbol{A}]\left[\boldsymbol{\pi} - q\boldsymbol{A} - \frac{1}{2}[\boldsymbol{\pi} - q\boldsymbol{A}]\right] + qU \\
&= \frac{1}{2m}[\boldsymbol{\pi} - q\boldsymbol{A}]^2 + qU.
\end{aligned}$$

The total energy should be

$$\frac{1}{2m}\boldsymbol{p}^2 + qU,$$

so the Hamilton function is not the total energy. Also, the rest mass would be missing, but that is another story.

1.3 Einstein-Lorentz-equation

1.3.1 Problem summary

The Poisson bracket to evaluate is

$$\dot{\boldsymbol{\pi}} = \{\boldsymbol{\pi}, H\} = \frac{\partial \boldsymbol{\pi}}{\partial x^j}\frac{\partial H}{\partial \pi_j} - \frac{\partial \boldsymbol{\pi}}{\partial \pi_j}\frac{\partial H}{\partial x^j}. \tag{1}$$

We will do this in small parts since there are a lot of terms here. For convenience, these are the momenta and Hamilton function again:

$$\pi_i = m\dot{x}_i + qA_i, \quad H = \frac{1}{2m}[\boldsymbol{\pi} - q\boldsymbol{A}]^2 + qU.$$

1.3.2 The parts

Left side The left side of the equation (1) is

$$\dot{\pi}_i = m\ddot{x}_i + q\dot{A}_i.$$

First part The first partial derivative in equation (1) is

$$\frac{\partial \pi_i}{\partial x^j} = \frac{\partial}{\partial x^j}\left[m\dot{x}_i + qA_i(x)\right] = q\frac{\partial A_i}{\partial x^j}.$$

Second part Now the partial derivative of the Hamilton function is needed:

$$\frac{\partial H}{\partial \pi_j} = \frac{1}{2m}\frac{\partial}{\partial \pi_j}[\pi_k - qA_k][\pi^k - qA^k] = \frac{\pi_j}{m} - \frac{q}{m}A_j.$$

Third part The next one is simply

$$\frac{\partial \pi_i}{\partial \pi_j} = \delta_i^j.$$

Fourth part The last partial derivative requires the most work:

$$\frac{\partial H}{\partial x^j} = \frac{1}{2m}\frac{\partial}{\partial x^j}\left[[\boldsymbol{\pi} - q\boldsymbol{A}]^2 + qU\right].$$

We expand the square, which is a scalar product, into two brackets with summation convention:

$$= \frac{1}{2m}\frac{\partial}{\partial x^j}\left[\pi_i - qA_i\right]\left[\pi^i - qA^i\right] + q\frac{\partial U}{\partial x^j}.$$

Using the product rule we can cancel the $1/2$ in front and apply the derivatives to the first bracket:

$$= \frac{1}{m}\left[\frac{\partial \pi_i}{\partial x^j} - q\frac{\partial A_i}{\partial x^j}\right]\left[\pi^i - qA^i\right] + q\frac{\partial U}{\partial x^j}.$$

We can now insert the derivatives of $\boldsymbol{\pi}$ since we have calculated them earlier on. We also factored out a q to the front:

$$= \frac{q}{m}\left[\frac{\partial A_i}{\partial x^j} - \frac{\partial A_i}{\partial x^j}\right]\left[\pi^i - qA^i\right] + q\frac{\partial U}{\partial x^j}.$$

This way, it is easy to see that the whole expression simplifies to the scalar potential term:

$$= q\frac{\partial U}{\partial x^j}.$$

This vanishing of the first part can also be made plausible when one recalls that

$$\dot{x}_i = \frac{1}{m}[\pi_i - qA_i].$$

From that,

$$\frac{\partial \dot{x}^i}{\partial x^j} = 0$$

can be understood faster.

1.3.3 Combined equation

Now that we have the parts together, we can put it into a single equation:

$$m\ddot{x}_i - q\dot{A}_i = q\frac{\partial A_i}{\partial x^j}\left[\frac{\pi_j}{m} + \frac{q}{m}A_j\right] - \delta_i^j q\frac{\partial U}{\partial x^j}.$$

We start by putting the $\dot{A}$ term to the right. Then we extract a factor $1/m$ out of the bracket:

$$\iff m\ddot{x}_i = \frac{q}{m}\frac{\partial A_i}{\partial x^j}\left[\pi_j - qA_j\right] - \delta_i^j q\frac{\partial U}{\partial x^j} - q\dot{A}_i.$$

The right side is just $\dot{p}_j$, the linear momentum. On the right side, we can insert the velocity for the bracket. We also take care of the δ finally:

$$\iff \dot{p}_i = q\frac{\partial A_i}{\partial x^j}\dot{x}_j - q\frac{\partial U}{\partial x^i} - q\dot{A}_i.$$

We factor out the q and rearrange the summands:

$$\iff \dot{p}_i = q\left[-\frac{\partial U}{\partial x^i} - \dot{A}_i + \frac{\partial A_i}{\partial x^j}\dot{x}_j\right].$$

We now use the second relation. The proof is at the end of this subsection. The equation now is

$$\iff \dot{p}_i = q\left[-\frac{\partial U}{\partial x^i} - \left[\frac{\partial A_i}{\partial t} + \dot{x}^j\frac{\partial A_i}{\partial x^j}\right] + \frac{\partial A_i}{\partial x^j}\dot{x}_j\right]$$
$$\iff \dot{p}_i = q\left[-\frac{\partial U}{\partial x^i} - \frac{\partial A_i}{\partial t}\right].$$

So far, this has not worked out to be the solution given on the problem set. I, MU, assume that I overlooked some part where I had to use product rule or so.

1.3.4 Proof of relations

The first identity can be shown with index notation.

Proof. We start in index notation:

$$[\dot{\boldsymbol{x}} \times [\boldsymbol{\nabla} \times \boldsymbol{A}]]_i = \epsilon_{ijk} \dot{x}_j \epsilon_{kmn} \partial_m A_n.$$

The ϵ commute to

$$= \epsilon_{ijk} \epsilon_{kmn} \dot{x}_j \partial_m A_n.$$

We do a cyclic permutation in the indices which does not change the value.

$$= \epsilon_{ijk} \epsilon_{mnk} \dot{x}_j \partial_m A_n.$$

Now we can contract the two Levi-Civita-symbols and obtain

$$= [\delta_{im} \delta_{jn} - \delta_{in} \delta_{jm}] \dot{x}_j \partial_m A_n.$$

Applying those to the remainder gives us less indices:

$$= \dot{x}_j \partial_i A_j - \dot{x}_j \partial_j A_i.$$

In order for the derivative appearing in front of the $\dot{x}_j$ we would need to subtract the term that the product rule would introduce. However, that term is zero in this case since $\dot{x}_j$ does not explicitly depend on x_i. The second summand in the above line can already be written in vector notation again. We obtain

$$= \partial_i \dot{x}_j A_j - [[\dot{\boldsymbol{x}} \boldsymbol{\nabla}] \boldsymbol{A}]_i \,.$$

Now we can write the first summand in vectorial notation as well:

$$= [\boldsymbol{\nabla} \dot{\boldsymbol{x}} \boldsymbol{A} - [\dot{\boldsymbol{x}} \boldsymbol{\nabla}] \boldsymbol{A}]_i \,.$$

That is the right side of the identity on the problem set, just with slightly different notation. □

There is still the proof of the second relation left.

Proof.

$$\dot{A}_i = \frac{\partial A_i}{\partial t} + \frac{\partial A_i}{\partial x^j} \frac{\partial x^j}{\partial t}.$$

Since the trajectories only depend on the time, that last derivative is a total one. We can therefore write it as $\dot{x}^j$.

$$= \frac{\partial A_i}{\partial t} + \frac{\partial A_i}{\partial x^j} \dot{x}^j.$$

We can also write this in a suggestive way like this:

$$= \frac{\partial A_i}{\partial t} + \dot{x}^j \frac{\partial}{\partial x^j} A_i.$$

Now one can see the whole vector identity:

$$\dot{\boldsymbol{A}} = \frac{\partial \boldsymbol{A}}{\partial t} + [\dot{\boldsymbol{x}} \boldsymbol{\nabla}] \boldsymbol{A}.$$

□

1.4 Analogy in quantum mechanics

In quantum mechanics, the commutator

$$[x^i, p_j] = \mathrm{i}\hbar \delta^i_j$$

is expected. In classical mechanics, the Poisson bracket

$$\{x^i, \pi_j\} = \delta^i_j$$

should hold for the canonical coordinates.

This problem might be solved by comparing $\{\boldsymbol{x}, \boldsymbol{p}\}$ with $\{\boldsymbol{x}, \boldsymbol{\pi}\}$. We got that δ^i_j in both cases, so we are not sure whether this is really the right way to handle this problem.

2 Charge conservation

2.1 Current density

The probability current density, which is proportional to the electric current density (omit q) can be derived by introducing the continuity equation and constructing the probability current density in a way such that it fulfils the continuity equation. Since one has to show that said equation is fulfilled in the next part of this problem, this is not the way to go.

From classical electrodynamics, the current density is defined as $\boldsymbol{j} := \boldsymbol{v}\rho$ where $\boldsymbol{v}$ is velocity field. Due to the uncertainty relation, it is impossible to give an exact $\boldsymbol{v}(\boldsymbol{x})$ which would proportional to $\boldsymbol{p}(\boldsymbol{x})$, since we are only dealing with non-relativistic quantum mechanics.

So frankly, we have no idea what we are supposed to do in this part of the problem.

2.2 Satisfaction of the continuity equation

The Schrödinger equation says in a compact notation:

$$\mathrm{i}\hbar \partial_0 \psi = H\psi.$$

The complex conjugate of this gives

$$-i\hbar\partial_0\psi^* = \psi^* H^*.$$

From that, we can write down the partial derivatives:

$$\dot{\psi} = -\frac{i}{\hbar}H\psi, \quad \dot{\psi}^* = \frac{i}{\hbar}H^*\psi^*.$$

We now start with the time derivative of ϱ in order to match it against the divergence of $\boldsymbol{j}$ later on.

$$\frac{\partial \varrho}{\partial t} = q\frac{\partial}{\partial t}\psi^*\psi$$

The first steps needs the product rule:

$$= q\left[\dot{\psi}^*\psi + \psi^*\dot{\psi}\right].$$

Then we can use the Schrödinger equation to give the time derivative of the wavefunction:

$$= \frac{iq}{\hbar}\left[\psi H^*\psi^* - \psi^* H\psi\right].$$

Factoring out a minus sign lets us write this in the notation that is introduced in the first part of this problem.

$$= -\frac{iq}{\hbar}\left[\psi^* H\psi - \text{h.c.}\right]$$

We insert the full hamiltonian:

$$= -\frac{iq}{\hbar}\left[\psi^*\left[\frac{1}{2m}[\boldsymbol{p} - q\boldsymbol{A}]^2 + qU\right]\psi - \text{h.c.}\right].$$

The part qU of the Hamiltonian is real, such that the subtraction of the hermitean conjugate will eliminate it. We therefore drop it and leave only

$$= -\frac{iq}{\hbar}\left[\psi^*\frac{1}{2m}[\boldsymbol{p} - q\boldsymbol{A}]^2\psi - \text{h.c.}\right].$$
$$= -\frac{iq}{2m\hbar}\left[\psi^*[\boldsymbol{p}^2 - q\boldsymbol{p}\boldsymbol{A} - q\boldsymbol{A}\boldsymbol{p} + q^2\boldsymbol{A}^2]\psi - \text{h.c.}\right].$$

By using the real/imaginary argument again, we can say that $\boldsymbol{p}^2$ and $\boldsymbol{A}^2$ vanish since they are purely real.

$$= \frac{iq^2}{2m\hbar}\left[\psi^*[\boldsymbol{p}\boldsymbol{A} + \boldsymbol{A}\boldsymbol{p}]\psi\right].$$

We insert $\boldsymbol{p} = -\mathrm{i}\hbar\boldsymbol{\nabla}$.

$$= \frac{q^2}{2m}\left[\psi^*[\boldsymbol{\nabla}\boldsymbol{A} + \boldsymbol{A}\boldsymbol{\nabla}]\psi\right].$$

The commutator of $\boldsymbol{A}$ and $\boldsymbol{\nabla}$ is

$$[\boldsymbol{\nabla}, \boldsymbol{A}] = \boldsymbol{\nabla}\boldsymbol{A}.$$

This can be seen by applying it to a wave function:

$$\boldsymbol{\nabla}\boldsymbol{A}\psi - \boldsymbol{A}\boldsymbol{\nabla}\psi = [\boldsymbol{\nabla}\boldsymbol{A}]\psi + \boldsymbol{A}\boldsymbol{\nabla}\psi - \boldsymbol{A}\boldsymbol{\nabla}\psi = [\boldsymbol{\nabla}\boldsymbol{A}]\psi.$$

Using the commutator we can simplify:

$$= \frac{q^2}{2m}\left[\psi^*[2\boldsymbol{A}\boldsymbol{\nabla} + [\boldsymbol{\nabla}\boldsymbol{A}]]\psi\right].$$

Now we write this in index notation, using the general relativity notation. There,

$$Z_{,i} := \frac{\partial Z}{\partial x^i}.$$

We end up with

$$= \frac{q^2}{2m}\left[2A^i\psi^*\psi_{,i} + \psi^* A^i_{,i}\psi\right]$$
$$= \frac{q^2}{2m}\boldsymbol{\nabla}\boldsymbol{A}\psi^*\psi.$$

Now we will tend to the current density $\boldsymbol{j}$. The continuity equation contains the divergence of the it, so we need to compute it. We start with the definition:

$$j^i = \frac{q}{2m}\left[\psi^*\left[-\mathrm{i}\hbar\partial^i - qA^i\right]\psi + \text{h.c.}\right]$$

We take the divergence. Here we have used a notation that is common in general relativity where there are lots of partial derivatives. Using that notation makes it possible to get everything into one line without huge brackets. Summation convention is again implied.

$$j^i_{,i} = \frac{q}{2m}\partial_i\left[\psi^*\left[-\mathrm{i}\hbar\partial^i - qA^i\right]\psi + \text{h.c.}\right]$$

Using product rule, we obtain more terms. We also but the hermitean conjugate to the very end outside of the brackets, the prefixed scalar factors are also implied.

$$= \frac{q}{2m}\left[\psi^*_{,i}\left[-\mathrm{i}\hbar\partial^i - qA^i\right]\psi + \psi^*\left[-\mathrm{i}\hbar\,\triangle - qA^i_{,i}\right]\psi + \psi^*\left[-\mathrm{i}\hbar\partial^i - qA^i\right]\psi_{,i}\right] + \text{h.c.}$$

The hermitean conjugate is added to this. Therefore, terms that are purely imaginary will be cancelled out. We do this step here to get rid of all the terms without A in it.

$$\begin{aligned}
&= -\frac{q^2}{2m}\left[\psi^*_{,i}A^i\psi + \psi^* A^i_{,i}\psi + \psi^* A^i \psi_{,i}\right] \\
&= -\frac{q^2}{2m}\left[A^i\partial_i\psi^*\psi + A^i_{,i}\psi^*\psi\right] \\
&= -\frac{q^2}{2m}\boldsymbol{\nabla}\boldsymbol{A}\psi^*\psi
\end{aligned}$$

The sum of the derived $\dot{\varrho}$ and this $\boldsymbol{\nabla}\boldsymbol{j}$ add up to zero, fulfilling the continuity equation.

2.3 Gauge invariance

ϱ does not change because the added phase for ψ has unit modulus.

For the current density, we have

$$\boldsymbol{j}' = \frac{q}{2m}\exp\left(-\mathrm{i}\frac{q}{\hbar}\lambda\right)\psi^*\left[-\mathrm{i}\hbar\boldsymbol{\nabla} - q\left[\boldsymbol{A} + [\boldsymbol{\nabla}\lambda]\right]\right]\exp\left(\mathrm{i}\frac{q}{\hbar}\lambda\right)\psi + \text{h.c.}.$$

Note that the first $\boldsymbol{\nabla}$ is supposed to act on the remainder of the line, the $[\boldsymbol{\nabla}\lambda]$ is supposed to be self-contained. It is a little hard to put the scope of the differential operators into this when not using the component notation of general relativity. Either way, there will be two additional terms here. One will come from the product and chain rule by the first $\boldsymbol{\nabla}$. The second will come from the gauge field itself.

$$= \boldsymbol{j} + \left[\frac{q}{2m}\psi^*\left[-\mathrm{i}\hbar\mathrm{i}\frac{q}{\hbar}\boldsymbol{\nabla}\lambda - q[\boldsymbol{\nabla}\lambda]\right]\psi + \text{h.c.}\right].$$

Cleaning up, it will become apparent that $\boldsymbol{j}$ is invariant under such gauge transformations.

$$\begin{aligned}
&= \boldsymbol{j} + \left[\frac{q}{2m}\psi^*\left[q[\boldsymbol{\nabla}\lambda] - q[\boldsymbol{\nabla}\lambda]\right]\psi + \text{h.c.}\right] \\
&= \boldsymbol{j}.
\end{aligned}$$

3 Some Gaussian integrals

3.1 First integral

3.1.1 The integral

We are asked to solve

$$\int_0^\infty \mathrm{d}x\, x\exp(-ax^2)$$

by calculating the indefinite integral first. So we do this by using substitution with

$$z := x^2, \quad \mathrm{d}z = 2x \, \mathrm{d}x.$$

Using that, we yield

$$\int \mathrm{d}x \, x \exp(-ax^2) = \frac{1}{2} \int \mathrm{d}z \, \exp(-az) = -\frac{1}{2a} \exp(-az).$$

Evaluating this at the boundary $[0, \infty)$ we obtain the result

$$\frac{1}{2a}.$$

3.1.2 Constraints on a

If the real part of a is negative, the integrand is not bounded any more and the function is not integrable any more. The result

$$\frac{1}{2a}$$

would turn negative for negative $\operatorname{Re} a$. However, the integrand itself would still be positive semi-definite. Therefore, this cannot be right. Unless one goes into the realm of complex magic where

$$\sum_{i=0}^{\infty} 2^{2i} = -\frac{1}{3}$$

can make some sense (Penrose 2005, p. 78).

3.2 2D Gaussian integral

$$\begin{aligned} |I_0(a)|^2 &= \int_{\infty}^{\infty} \mathrm{d}x \exp(-ax^2) \int_{\infty}^{\infty} \mathrm{d}y \exp(-ay^2) \\ &= \int_{\infty}^{\infty} \mathrm{d}x \int_{\infty}^{\infty} \mathrm{d}y \exp(-a[x^2 + y^2]) \end{aligned}$$

Now $x^2 + y^2 = r^2$ in polar coordinates. The measure of the integration, which can be derived from Gram's determinant of the metric tensor, is $r \, \mathrm{d}r \, \mathrm{d}\phi$.

$$= \int_0^{\infty} r \, \mathrm{d}r \int_0^{2\pi} \mathrm{d}\phi \exp(-ar^2)$$

Since the integrand does not depend on ϕ, we will get a simple scalar factor:

$$= 2\pi \int_0^\infty r \, \mathrm{d}r \exp(-ar^2).$$

Using the previously derived fact that this integral is $1/2a$ we can write down the result:

$$= \frac{\pi}{a}.$$

That was the square of the integral to be calculated, so the integral itself is

$$\sqrt{\frac{\pi}{a}}.$$

3.3 Third integral

We shall compute

$$I_2(a) = \int_{-\infty}^{\infty} \mathrm{d}x \, x^2 \exp(-ax^2).$$

We can obtain a x^2 from the exponential function via a differentiation:

$$= -\int_{-\infty}^{\infty} \mathrm{d}x \frac{\mathrm{d}}{\mathrm{d}a} \exp(-ax^2).$$

Using the Lebeque's theorem, without checking the prerequisites, we get

$$= -\frac{\mathrm{d}}{\mathrm{d}a} \int_{-\infty}^{\infty} \mathrm{d}x \exp(-ax^2).$$

We already solved that integral, so we get

$$= -\frac{\mathrm{d}}{\mathrm{d}a} \sqrt{\frac{\pi}{a}}.$$

One way of writing this would be

$$= \frac{1}{2} \sqrt{\frac{\pi}{a^3}}.$$

3.4 Fourth integral

First we note the following:

$$ax^2 + bx = \left[\sqrt{a} x + \frac{1}{2\sqrt{a}} b \right]^2 - \frac{b^2}{4a}.$$

The integral to compute is

$$I_0(a, b) = \int_{-\infty}^{\infty} \mathrm{d}x \exp(-ax^2 + bx).$$

We use the completion of the square we showed above:

$$= \int_{-\infty}^{\infty} \mathrm{d}x \exp\left(-\left[\sqrt{a}x + \frac{b}{2\sqrt{a}}\right]^2 + \frac{b^2}{4a}\right).$$

The constant term can be put in front of the integral:

$$= \exp\left(\frac{b^2}{4a}\right) \int_{-\infty}^{\infty} \mathrm{d}x \exp\left(-\left[\sqrt{a}x + \frac{b}{2\sqrt{a}}\right]^2\right).$$

Using a substitution of the integrand with a simple shift we can remove the

$$+\frac{b}{2\sqrt{a}}$$

part in the exponential function. Since it is a finite shift and the bounds are infinite, this will not change the value of the integral at all. Therefore, we use the same variable x and just drop the term linear in b. We get

$$= \exp\left(\frac{b^2}{4a}\right) \int_{-\infty}^{\infty} \mathrm{d}x \exp(-ax^2).$$

The integral is well known by now, we can just insert it and obtain the final result of

$$= \exp\left(\frac{b^2}{4a}\right) \sqrt{\frac{\pi}{a}}.$$

References

Penrose, Roger (2005). *Road to Reality*. 1. New York: Alfred A. Knopf. ISBN: 0-679-45443-8.