Prof. Dr. Stefan Hofmann Wintersemester 2018/19

Übungen zur Quantenmechanik (T2)

Übungsblatt 0, Besprechung vom 15.10.-20.10.

Dieses Übungsblatt dient der Wiederholung einiger relevanter Grundlagen aus vorherigen Vorlesungen. Falls Sie konzeptionelle Probleme haben, sollten Sie dies zum Anlass nehmen, die relevanten Themen zu wiederholen.

Gegeben sei die Matrix $M = \begin{pmatrix} 4 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & -4 \end{pmatrix}$.

(i) Bestimmen Sie die Eigenwerte und Eigenvektoren der Matrix M.

(ii) Diagonalisieren Sie M.

(iii) Berechnen Sie M^2 durch direkte Matrixmultiplikation und durch die Definition einer Matrixfunktion $f(M) := Uf(D)U^{-1}$, wobei $M = UDU^{-1}$, und D eine Diagonalmatrix ist.

(iv) Überzeugen Sie sich, dass M eine hermitesche Matrix ist, und berechnen Sie dessen Spur $\mathrm{tr}(M)$.

(v) Zeigen Sie, dass der Raum der hermiteschen, spurlosen $n \times n$ Matrizen versehen mit Matrixaddition und skalarer Multiplikation einen $\mathbb{R}$-Vektorraum bildet. Bilden diese Matrizen auch einen $\mathbb{C}$-Vektorraum?

Eine Basis dieses Vektorraumes bilden die Gell-Mann-Matrizen

$$\lambda_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad \lambda_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad \lambda_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\lambda_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \qquad \lambda_5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}$$

$$\lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \qquad \lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \qquad \lambda_8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}.$$

(vi) Zeigen Sie, dass für zwei hermitesche, spurlose Matrizen A, B die Abbildung $\langle A, B \rangle := \mathrm{tr}(AB)$ ein inneres Produkt auf dem Raum der hermiteschen, spurlosen Matrizen definiert.

(vii) Zeigen Sie, dass die Vektoren $\{e_i\}_{i \in I(8)}$ mit $e_i := \frac{1}{\sqrt{2}}\lambda_i$ orthonormal zueinander sind.

(viii) Finden Sie die Darstellung von M in der Basis $\{e_i\}_{i \in I(8)}$ durch Projektion auf die Basisvektoren.

Solution

(i) To find the eigenvalues, we compute $\det(M - \lambda I)$ and obtain, expanding the determinant

$$\det(M - \lambda I) = (4 - \lambda) \det \begin{pmatrix} -\lambda & 1 \\ 1 & -4 - \lambda \end{pmatrix} = 0 \tag{1}$$

so as expected, $\lambda_1 = 4$. The remaining determinant gives a quadratic equation in λ,

$$\lambda^2 + 4\lambda - 1 = 0, \tag{2}$$

which has the roots

$$\lambda_2 = -2 + \sqrt{5}, \tag{3}$$
$$\lambda_3 = -2 - \sqrt{5}. \tag{4}$$

The eigenvectors can be computed straightforwardly by first observing that $w_1 = (1, 0, 0)^T$, and from the second row of $M - \lambda_i I$ we can read off

$$w_2 = (0, -\lambda_3, 1)^T, \tag{5}$$
$$w_3 = (0, -\lambda_2, 1)^T. \tag{6}$$

Since M is Hermitean and the eigenvalues are non-degenerate, they are already orthogonal and we can simply normalise them to obtain an orthonormal basis v_1, v_2, v_3 with

$$v_1 = (1, 0, 0)^T \tag{7}$$
$$v_2 = \frac{1}{\sqrt{1+\lambda_3^2}}(0, -\lambda_3, 1)^T \tag{8}$$
$$v_3 = \frac{1}{\sqrt{1+\lambda_2^2}}(0, -\lambda_2, 1)^T. \tag{9}$$

(ii) We digaonalise M by finding the unitary Matrix U such that $M = UDU^\dagger$, where D is a diagonal matrix. Since we already have an orthonormal eigenbasis, we can find $U = (v_1, v_2, v_3)$, which gives, after noting that $(1 + \lambda_2^2)(1 + \lambda_3^2) = 20$, the matrix

$$U = \frac{1}{\sqrt{20}} \begin{pmatrix} \sqrt{20} & 0 & 0 \\ 0 & -\lambda_3\sqrt{1+\lambda_2^2} & -\lambda_2\sqrt{1+\lambda_3^2} \\ 0 & \sqrt{1+\lambda_2^2} & \sqrt{1+\lambda_3^2} \end{pmatrix} \tag{10}$$

After a straightforward computation we obtain

$$U^\dagger M U = \frac{1}{20} \begin{pmatrix} 20 \cdot 4 & 0 & 0 \\ 0 & (1+\lambda_2^2)(-2\lambda_3 - 4) & \sqrt{1+\lambda_2^2}\sqrt{1+\lambda_3^2}(-\lambda_2 - \lambda_3 - 4) \\ 0 & \sqrt{1+\lambda_2^2}\sqrt{1+\lambda_3^2}(-\lambda_2 - \lambda_3 - 4) & (1+\lambda_3^2)(-2\lambda_2 - 4) \end{pmatrix} \tag{11}$$

We can now use $\lambda_2 + \lambda_3 = -4$ to see that the off-diagonal elements vanish, and on the diagonal we compute

$$-2\lambda_3 - 4 = 2\sqrt{5} \tag{12}$$
$$-2\lambda_2 - 4 = -2\sqrt{5} \tag{13}$$

as well as

$$1 + \lambda_2^2 = 10 - 4\sqrt{5} = 2\sqrt{5}(-2 + \sqrt{5}) \tag{14}$$
$$1 + \lambda_3^2 = 10 + 4\sqrt{5} = 2\sqrt{5}(2 + \sqrt{5}) \tag{15}$$

to obtain in the diagonal slots $20 \cdot \lambda_{2/3}$, respectively. The diagonal matrix is thus given by

$$D = U^\dagger M U = \begin{pmatrix} 4 & 0 & 0 \\ 0 & -2+\sqrt{5} & 0 \\ 0 & 0 & -2-\sqrt{5} \end{pmatrix}. \tag{16}$$

(iii) Straightforward computation gives

$$M^2 = \begin{pmatrix} 16 & 0 & 0 \\ 0 & 1 & -4 \\ 0 & -4 & 17 \end{pmatrix} \tag{17}$$

We also note that

$$M^2 = U^\dagger D U U^\dagger D U = U^\dagger D^2 U \tag{18}$$

so indeed the definition given in the exercise agrees with M^2 and an explicit computation can show this as well.

(iv) A Hermitean matrix T satisfies $T^\dagger = T$ (where $T^\dagger$ denotes the Hermitean adjoint, i.e. transpose and complex-conjugate), so M is Hermitean. Furthemore, we evaluate $\operatorname{tr} M = 0$, so M is a Hermitean, traceless matrix.

(v) The space of Hermitean, traceless $n \times n$ matrices is a real vector space, since it contains the neutral element, the 0-matrix, and is closed under addition and scalar multiplication.

Note that it is not a complex vector space, since multiplication by i turns a Hermitian matrix into an anti-Hermitian one.

(vi) An inner product on a vector space V is a map $\langle \cdot, \cdot \rangle \colon V \times V \to \mathbb{C}$ which satisfies

a) positive-definiteness, i.e. for all $v \in V$ $\langle v, v\rangle \geq 0$ and $= 0$ only if $v = 0$.

b) linearity in the second slot, i.e. for all $u, v, w \in V$ and $\alpha, \beta \in \mathbb{C}$ we have

$$\langle u, \alpha v + \beta w\rangle = \alpha \langle u, v\rangle + \beta \langle u, w\rangle.$$

c) complex-conjugate symmetry, i.e. for all $u, v \in V$ we have $\overline{\langle u, v\rangle} = \langle v, u\rangle$.

We now show that $\operatorname{tr}(AB)$ satisfies all these properties. Note that in this case, $\operatorname{tr}(AB) = \operatorname{tr}(A^\dagger B)$, which is the standard definition of an inner product on matrix spaces.

a) Suppose now that we have a matrix A that is Hermitean and traceless. It must have at least one real eigenvalue that is non-zero, else it is the zero matrix. We can now compute

$$\operatorname{tr}(AA) = \operatorname{tr}(U D_A U^\dagger U D_A U^\dagger) = \operatorname{tr}(D_A^2) = \sum_i \lambda_i^2 > 0, \tag{19}$$

where we used that the trace is cyclic, the eigenvalues of Hermitean matrices are real and that A is not the zero matrix. So we satisfy positive-definiteness.

b) The trace is a linear map, so in particular we have for Hermitean matrices A, B, C and $\alpha, \beta \in \mathbb{C}$ that

$$\operatorname{tr}(A(\alpha B + \beta C)) = \alpha \operatorname{tr}(AB) + \beta \operatorname{tr}(AC), \tag{20}$$

which shows linearity in the second slot.

c) For Hermitean matrices A, B, we compute

$$\overline{\operatorname{tr}(AB)} = \operatorname{tr}((AB)^\dagger) = \operatorname{tr}(B^\dagger A^\dagger) = \operatorname{tr}(BA). \tag{21}$$

(vii) Explicit computation shows that $\operatorname{tr}(\lambda_i \lambda_j) = 2\delta_{ij}$, so indeed $\frac{1}{\sqrt{2}}\lambda_i$ are orthonormal.

(viii) We can project on the basis using the scalar product, by writing

$$v = \sum_i \langle e_i, v\rangle \, e_i. \tag{22}$$

We can see or compute the coefficients and obtain

$$M = 2\lambda_3 + \lambda_6 + 2\sqrt{3}\lambda_8 = 2\sqrt{2}e_3 + \sqrt{2}e_6 + 2\sqrt{6}e_8. \tag{23}$$

Aufgabe 2 – Funktionenräume

(i) Betrachten Sie den Funktionenraum

$$\mathscr{L}^2([0,1], \mathbb{R}) := \{f \colon [0,1] \to \mathbb{R} : \int_0^1 \mathrm{d}x \, |f(x)|^2 < \infty \wedge f(x=0) = f(x=1) = 0\}.$$

Zeigen Sie, dass $\mathscr{L}^2$ zusammen mit punktweiser Addition

$$\oplus \colon \mathscr{L}^2 \times \mathscr{L}^2 \to \mathscr{L}^2 \tag{24}$$

$$(f, g) \mapsto f \oplus g, \text{ so dass } (f \oplus g)(x) := f(x) +_{\mathbb{R}} g(x) \tag{25}$$

und skalarer Multiplikation

$$\odot \colon \mathbb{R} \times \mathscr{L}^2 \to \mathscr{L}^2 \tag{26}$$

$$(\lambda, f) \mapsto \lambda \odot f, \text{ so dass } (\lambda \odot f)(x) := \lambda \cdot_{\mathbb{R}} f(x) \tag{27}$$

einen $\mathbb{R}$-Vektorraum bildet.
Später werden wir Vektoraddition und skalare Multiplikation mit + respektive · bezeichnen, hier soll nur klargemacht werden, dass es sich bei diesen Operationen um Vektoroperationen und nicht um Körperoperationen handelt.

(ii) Zeigen Sie, dass durch $\langle f, g\rangle = \int_0^1 \mathrm{d}x\, f(x)g(x)$ eine positiv-semidefinite Bilinearform definiert wird. Warum ist diese nicht positiv-definit? Welche Schritte können Sie unternehmen, um einen Vektorraum mit einem inneren Produkt zu erhalten?

(iii) Betrachten Sie nun den Unterraum der stetigen Funktionen auf $[0, 1]$. Die Funktionen $\{\sin(\pi n x)\}_{n\in\mathbb{N}}$ bilden eine orthogonale Basis dieses Unterraums. Entwickeln Sie die folgenden Elemente von $\mathscr{L}^2([0, 1], \mathbb{R})$ in dieser Basis:

$$f_1(x) = \sin(\pi x), \quad f_2(x) = \sin^2(\pi x), \quad f_3(x) = x^2 - x$$

Solution

(i) A $\mathbb{K}$-vector space is a 4-tuple $(\mathbb{K}, V, \oplus, \odot)$ consisting of a field $\mathbb{K}$, a set V, vector addition $\oplus$ and scalar multiplication $\odot$ defined as

$$\oplus\colon V \times V \to V, \tag{28}$$
$$\odot\colon \mathbb{K} \times V \to V, \tag{29}$$

satisfying the properties (CANI-ADDU)

a) Commutativity of addition: For vectors $u, v \in V$ we have

$$u \oplus v = v \oplus u.$$

b) Associativity of addition: For vectors $u, v, w \in V$ we have

$$u \oplus (v \oplus w) = (u \oplus v) \oplus w = u \oplus v \oplus w.$$

c) Neutral Element of addition: There exists an element e in V such that for all $v \in V$ we have

$$e \oplus v = v.$$

d) Inverse Element of addition: To each vector $v \in V$ there exists an element $w \in V$ such that

$$w \oplus v = e.$$

e) Associativity: For each $\alpha, \beta \in \mathbb{K}$ and $v \in V$ we have

$$\alpha \odot (\beta \odot v) = (\alpha \cdot \beta) \odot v.$$

f) Distributivity: For each $\alpha \in \mathbb{K}$ and $u, v \in V$ we have

$$\alpha \odot (v \oplus w) = \alpha \odot v \oplus \alpha \odot w.$$

g) Distributivity: For each $\alpha, \beta \in \mathbb{K}$ and $v \in V$ we have

$$(\alpha + \beta) \odot v = \alpha \odot v \oplus \beta \odot v.$$

h) Unit element: For the unit element $1 \in \mathbb{K}$ w.r.t multiplication, we have

$$1 \odot v = v.$$

By explicit computation and using the known properties of $+, \cdot$ in $\mathbb{R}$ we see that the function space $\mathbb{L}^2([0, 1], \mathbb{R})$ is indeed a $\mathbb{R}$-vector space.

(ii) For a real scalar product, we need bilinearity, positive-definiteness and symmetry. Clearly, the integral is linear and multiplication in $\mathbb{R}$ is symmetric, so we only need to check positive-definiteness. We see that

$$\langle f, f\rangle = \int \mathrm{d}x f(x)^2 \geq 0. \tag{30}$$

However, there may be functions which are not identical to the zero-function, but that are almost everywhere zero, i.e. non-zero only on a set of Lebesgue-measure zero, which destroys positive-definiteness.

(iii) We will use the trigonometric identities

$$\sin(\alpha+\beta) = \sin\alpha\cos\beta + \sin\beta\cos\alpha \tag{31}$$

$$\cos(\alpha+\beta) = \cos\alpha\cos\beta - \sin\alpha\sin\beta \tag{32}$$

to derive

$$\sin\alpha\sin\beta = \frac{1}{2}(\cos(\alpha-\beta) - \cos(\alpha+\beta)) \tag{33}$$

$$\cos\alpha\cos\beta = \frac{1}{2}(\cos(\alpha+\beta) + \cos(\alpha-\beta)) \tag{34}$$

$$\sin\alpha\cos\beta = \frac{1}{2}(\sin(\alpha+\beta) + \sin(\alpha-\beta)). \tag{35}$$

This will simplify the calculations a lot.
We can compute the coefficients by noting that

$$\boldsymbol{v} = c_i e_i \Rightarrow c_i \left|e_i\right|^2 = \langle e_i, v\rangle,$$

and since the vectors are not orthonormal, we have $\boldsymbol{e_i}^2 = \frac{1}{2}$. Clearly $f_1 = e_1$.
For f_2, first note that $\sin^2(\pi x)$ is symmetric w.r.t $x = \frac{1}{2}$, whereas $\sin(n\pi x)$ with even n, $n \neq 0$ is antisymmetric w.r.t this point. So we can already see that all coefficients $\{a_n\}_{n\in 2\mathbb{N}}$ vanish. For odd n, we can use the above relations. We have

$$\int \mathrm{d}x\ \sin^2(\pi x)\sin(n\pi x) = \int \mathrm{d}x\ \frac{1}{2}\left(\cos(0) - \cos(2\pi x)\right)\sin(n\pi x) \tag{36}$$

$$= \frac{1}{n\pi} - \frac{1}{2}\int \mathrm{d}x\ \cos(2\pi x)\sin(n\pi x) \tag{37}$$

$$= \frac{1}{n\pi} - \frac{1}{4}\int \mathrm{d}x\ \left(\sin((n+2)\pi x) + \sin((n-2)\pi x)\right) \tag{38}$$

$$= \frac{1}{n\pi} - \frac{1}{2(n+2)\pi} - \frac{1}{2(n-2)\pi}. \tag{39}$$

To see that this holds for all n, we can show this inductively. So the expansion in the basis is given by

$$a_n = \begin{cases} 2\left(\frac{1}{n\pi} - \frac{1}{2(n+2)\pi} - \frac{1}{2(n-2)\pi}\right), & \text{for } n \text{ odd,} \\ 0, & \text{for } n \text{ even.} \end{cases} \tag{40}$$

To find the expansion of f_3, we use integration by parts. First we compute

$$\int \mathrm{d}x\ x^2\sin(n\pi x) = -\frac{\cos(n\pi)}{n\pi} + \int \mathrm{d}x\ 2x\frac{\cos(n\pi x)}{n\pi} \tag{41}$$

$$= -\frac{\cos(n\pi)}{n\pi} - \int \mathrm{d}x\ 2\frac{\sin(n\pi x)}{(n\pi)^3} \tag{42}$$

$$= -\frac{\cos(n\pi)}{n\pi} - \frac{2}{(n\pi)^3} + \frac{2\cos(n\pi))}{(n\pi)^3}. \tag{43}$$

Similarly, we have

$$\int \mathrm{d}x\ x\sin(n\pi x) = -\frac{cos(n\pi)}{n\pi}. \tag{44}$$

So in total we get

$$a_n = -2\left(\frac{2}{(n\pi)^3} + (-1)^n\frac{2}{(n\pi)^3}\right). \tag{45}$$

As expected, for even n, the coefficients vanish by symmetry. We can simplify this to be

$$a_n = \begin{cases} -\frac{8}{(n\pi)^3}, & \text{for } n \text{ odd,} \\ 0, & \text{for } n \text{ even.} \end{cases} \tag{46}$$

Aufgabe 3 – Fourier-Transformationen

Wir betrachten im Folgenden den Raum der glatten Funktionen mit kompaktem Träger (wir definieren für eine Funktion $f\colon \mathbb{R} \to \mathbb{R}$ den Träger als $\text{Träger}(f) := \{x \in \mathbb{R}\colon f(x) \neq 0\}$), bezeichnet als $C_0^\infty(\mathbb{R})$. Wir definieren die Fourier-Transformation einer Funktion $f \in C_0^\infty(\mathbb{R})$ als

$$\hat{f}(k) := \int_{\mathbb{R}} \mathrm{d}x\, f(x) e^{-ikx}. \tag{47}$$

(i) Bestimmen Sie die inverse Fourier-Transformation, d.h. drücken Sie $f(x)$ durch $\hat{f}(k)$ aus. Die folgende Darstellung der Delta-Distribution können Sie dabei benutzen:

$$\int_{-\infty}^{\infty} \mathrm{d}x\, e^{ikx} = 2\pi\delta(k) \tag{48}$$

(ii) Zeigen Sie die folgenden Identitäten:

a)

$$\int_{-\infty}^{\infty} \mathrm{d}x\, |f(x)|^2 = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}k\, \left|\hat{f}(k)\right|^2, \tag{49}$$

b)

$$\widehat{f^{(n)}}(k) = (ik)^n \hat{f}(k), \tag{50}$$

c)

$$\hat{f}_a(k) = \frac{1}{|a|}\hat{f}\left(\frac{k}{a}\right), \text{ wobei } f_a(x) = f(ax) \text{ und } a \in \mathbb{R}. \tag{51}$$

Wir können diese Fourier-Transformation auf einen größeren Raum von Funktionen erweitern, das genaue Vorgehen hierfür geben wir an dieser Stelle nicht an. Im Folgenden können Sie also Ihre Kenntnisse der Fouriertransformation benutzen und müssen sich keine Sorgen um Konvergenz von Integralen machen, es lässt sich alles wohldefinieren.

(iii) Bestimmen Sie die Fourier-Transformierten der folgenden Funktionen (für $a \in \mathbb{R}^+$):

a) $f_1(x) = e^{-ax^2}$

b) $f_2(x) = \sin(ax)$

c) $f_3(x) = \dfrac{1}{x^2 + a^2}$

Solution

(i) We make an ansatz for the inverse Fourier transformation

$$\check{\hat{f}}(x) = \frac{1}{2\pi} \int \mathrm{d}k\, \hat{f}(k) e^{ikx}, \tag{52}$$

and compute this directly

$$\begin{aligned} \check{\hat{f}}(x) &= \frac{1}{2\pi} \int \mathrm{d}k\, e^{ikx} \int \mathrm{d}y\, f(y) e^{-iky} && (53)\\ &= \frac{1}{2\pi} \int \mathrm{d}k\, \mathrm{d}y\, f(y) e^{ik(x-y)} && (54)\\ &= f(x), && (55) \end{aligned}$$

where we interchanged the order of integration and used the delta-distribution to get the last line.

(ii) a) We simply use the Fourier transformation to obtain

$$\int \mathrm{d}x\ |f(x)|^2 = \int \mathrm{d}x \frac{\mathrm{d}k}{2\pi}\frac{\mathrm{d}q}{2\pi}\overline{\hat{f}(k)}e^{-ikx}\hat{f}(q)e^{iqx} \tag{56}$$

$$= \int \frac{\mathrm{d}k}{2\pi}\frac{\mathrm{d}q}{2\pi}\overline{\hat{f}(k)}\hat{f}(q)2\pi\delta(k-q) \tag{57}$$

$$= \int \frac{\mathrm{d}k}{2\pi}\left|\hat{f}(k)\right|^2, \tag{58}$$

where we interchanged the order of integration in the second line and used the representation of the delta-distribution given in Eq. (48).

b) Since f is smooth, we can compute arbitrarily high orders of derivatives. We compute first $n=1$. Consider the Fourier-transformation

$$\widehat{f'}(k) = \int \mathrm{d}x\, f'(x)e^{-ikx} \tag{59}$$

$$= f(x)e^{-ikx}\big|_{-\infty}^{\infty} - \int \mathrm{d}x\, f(x)(-ik)e^{-ikx} \tag{60}$$

$$= ik\int \mathrm{d}x\, f(x)e^{-ikx} \tag{61}$$

$$= ik\hat{f}(k), \tag{62}$$

where we used that f has compact support, so the boundary term evaluates to zero. We can now prove the identity for arbitrary $n \in \mathbb{N}$ inductively. Consider $n \to n+1$:

$$\widehat{f^{(n+1)}}(k) = \int \mathrm{d}x\, \frac{\mathrm{d}^{n+1}f}{\mathrm{d}x^{n+1}}(x)e^{-ikx} \tag{63}$$

$$= \frac{\mathrm{d}^n f}{\mathrm{d}x^n}(x)e^{-ikx}\bigg|_{-\infty}^{\infty} - ik\int \mathrm{d}x\, \frac{\mathrm{d}^x n}{\mathrm{d}f(x)^x}e^{-ikx} \tag{64}$$

$$= ik\widehat{f^{(n)}}(k) \tag{65}$$

$$= ik(ik)^n\hat{f}(k) \tag{66}$$

$$= (ik)^{n+1}\hat{f}(k), \tag{67}$$

where we used in the third line that the derivatives of f also have compact support and the induction hypothesis in the fourth line.

c) This follows by rescaling the measure in the integral. We have

$$\hat{f}_a(k) = \int \mathrm{d}x\, f(ax)e^{-ikx} \tag{68}$$

$$= \int \frac{\mathrm{d}x}{|a|} f(x)e^{-ik\frac{x}{a}} \tag{69}$$

$$= \frac{1}{|a|}\hat{f}\left(\frac{k}{a}\right) \tag{70}$$

$$\tag{71}$$

(iii) a) We first show that the Gaussian integral gives

$$I(a) = \int_{-\infty}^{\infty} \mathrm{d}x\, e^{-ax^2} = \sqrt{\frac{\pi}{a}}. \tag{72}$$

To see this, we compute first the square of the integral

$$I^2(a) = \int_{-\infty}^{\infty}\mathrm{d}x\int_{-\infty}^{\infty}\mathrm{d}y\, e^{-a(x^2+y^2)} \tag{73}$$

$$= \int_0^{\infty}\mathrm{d}r\int_0^{2\pi} r\mathrm{d}\varphi\, e^{-ar^2} \tag{74}$$

$$= 2\pi\int_0^{\infty}\mathrm{d}r\, -\frac{1}{2a}\frac{\partial}{\partial r}e^{-ar^2} \tag{75}$$

$$= \frac{\pi}{a}, \tag{76}$$

from which we can conclude that $I(a) = \sqrt{\frac{\pi}{a}}$. With this we can now compute the Fourier transform. We have

$$\hat{f}_1(k) = \int \mathrm{d}x\, e^{-ax^2} e^{-ikx} \tag{77}$$
$$= \int \mathrm{d}x\, e^{-ax^2-ikx} \tag{78}$$
$$= \int \mathrm{d}x\, e^{-a(x+\frac{ik}{2a})^2-\frac{k^2}{4a}} \tag{79}$$
$$= e^{-\frac{k^2}{4a}} \int \mathrm{d}x\, e^{-a(x+\frac{ik}{2a})^2} \tag{80}$$
$$= \sqrt{\frac{\pi}{a}} e^{-\frac{k^2}{4a}}. \tag{81}$$

b) We compute

$$\hat{f}_2(k) = \int \mathrm{d}x\, \sin(ax) e^{-ikx} \tag{82}$$
$$= \int \mathrm{d}x\, \frac{1}{2i}\left(e^{iax} - e^{-iax}\right) e^{-ikx} \tag{83}$$
$$= \frac{1}{2i}\left(\int \mathrm{d}x\, e^{ix(a-k)} - \int \mathrm{d}x\, e^{-ix(a+k)}\right) \tag{84}$$
$$= -i\pi\left(\delta(a-k) - \delta(a+k)\right). \tag{85}$$

c) We have

$$\hat{f}_3 = \int \mathrm{d}x\, \frac{e^{-ikx}}{x^2+a^2} = \int \mathrm{d}x\, \frac{e^{-ikx}}{(x+ia)(x-ia)}. \tag{86}$$

To compute this, we use contour integration. Suppose that $k > 0$, then we have to close the contour in the lower half-plane. There is one pole in the lower half-plane at $x = -ia$. The residuum of this pole is given by $\mathrm{Res}(f_3, -ia) = \pi\frac{e^{-ka}}{-2ia}$. The integral thus evaluates

$$\int \mathrm{d}x\, \frac{e^{-ikx}}{(x+ia)(x-ia)} = -2\pi i\pi\frac{e^{-ka}}{-2ia} = \pi\frac{e^{-ka}}{a}. \tag{87}$$

If $k < 0$, we have to close the contour in the upper half-plane, and we obtain

$$\int \mathrm{d}x\, \frac{e^{-ikx}}{(x+ia)(x-ia)} = 2\pi i\pi\frac{e^{ka}}{2ia} = \pi\frac{e^{-|k|a}}{a}. \tag{88}$$

We conclude that the Fourier-transformed function is given by

$$\hat{f}_3(k) = \pi\frac{e^{-|k|a}}{a}. \tag{89}$$

Aufgabe 4 – Hamilton-Formalismus

(i) Leiten Sie durch Variation der Wirkung $S = \int \mathrm{d}t\, L(q, \dot{q}(q,p)) = \int \mathrm{d}t\, p\dot{q}(q,p) - H(q,p)$ die Hamiltonschen Gleichungen her.

(ii) Betrachten Sie ein System dessen Dynamik invariant ist unter der Transformation $q \to q + \Delta q$. Welche Erhaltungsgröße ergibt sich hieraus? Welche resultiert aus der Invarianz unter $t \to t + \Delta t$? Begründen Sie durch explizite Rechnung!

(iii) Bestimmen Sie die Erhaltungsgrößen die sich aus den folgenden Lagrange-Funktionen ergeben:

$$L = \frac{m}{2}(\dot{x}^2 + \dot{y}^2) - \frac{\alpha}{x^2+y^2}$$
$$L = \frac{m}{2}\dot{r}^2 + \frac{m}{2}r^2\dot{\phi}^2 - \alpha(t) r\cos(\phi)$$

(iv) Zeigen Sie dass für eine beliebige Funktion $O(q(t), p(t), t)$ die folgenden Identitäten gelten:

$$\frac{\mathrm{d}}{\mathrm{d}t} O(q(t), p(t), t) = \{O, H\} + \frac{\partial O}{\partial t}$$
$$\frac{\mathrm{d}}{\mathrm{d}q} O(q(t), p(t), t) = \{O, p\}$$
$$\frac{\mathrm{d}}{\mathrm{d}p} O(q(t), p(t), t) = -\{O, q\}$$

(v) Bestimmen Sie für die folgende Lagrange-/Hamilton-Funktion die dazugehörige Hamilton-/Lagrange-Funktion:

$$L(q, \dot{q}) = \frac{\mu}{4}\dot{q}^4 - aq\dot{q} - \frac{\omega}{2}q^2$$
$$H(q, p) = \frac{1}{2}(\mu p - \lambda q)^2$$

(vi) Betrachten Sie ein Teilchen der Masse m im eindimensionalen Oszillatorpotential $V(q) = \frac{m\omega^2}{2}q^2$. Bestimmen Sie $q(t)$ und $p(t)$ und skizzieren Sie diese im Phasenraum. Beschreiben Sie anschließend wie Sie Ihre Skizze anpassen müssten um zwei Teilchen in diesem Potential darstellen zu können.

Solution

(i) We perform the variation

$$\delta S = \int \mathrm{d}t\, \delta p \dot{q} + p\delta\dot{q} - \delta H \tag{90}$$
$$= \int \mathrm{d}t\, \delta p \left(\dot{q} - \frac{\partial H}{\partial p}\right) + \left(p\delta\dot{q} - \frac{\partial H}{\partial q}\delta q\right) \tag{91}$$
$$= \int \mathrm{d}t\, \delta p \left(\dot{q} - \frac{\partial H}{\partial p}\right) + \left(-\dot{p} - \frac{\partial H}{\partial q}\right)\delta q, \tag{92}$$

from which we can read off the equations of motion

$$\frac{\partial H}{\partial p} = \dot{q} \tag{93}$$
$$\frac{\partial H}{\partial q} = -\dot{p}. \tag{94}$$

(ii) The action is given by

$$S = \int \mathrm{d}t\, L(q, \dot{q}, t). \tag{95}$$

If the action is invariant under a transformation $q \to q + \delta q$, the Lagrangian is invariant up to a total derivative. This means that

$$\delta L = \frac{\mathrm{d}}{\mathrm{d}t}K \tag{96}$$

for some function K. We compute the variation of L directly and get

$$\delta L = \frac{\partial L}{\partial q}\delta q + \frac{\partial L}{\partial \dot{q}}\delta\dot{q} \tag{97}$$

Combining both variations and using the equation of motion, we find a conserved charge

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}}\delta q - K\right) = 0. \tag{98}$$

Since the action is translationally invariant, we have $\frac{\partial L}{\partial q} = 0$, as well as $K = 0$. We then have for a translation $\delta q = c = \text{const}$, and the corresponding conserved charge is the momentum $p_q = \frac{\partial L}{\partial \dot{q}}$.
For time-translations $t \to t + \delta t$, we have $q(t) \to q'(t') = q(t)$ which corresponds to a transformation

$$q(t) \to q'(t) = q(t) - \dot{q}\delta t. \tag{99}$$

The Lagrangian changes by $\delta L = \frac{\mathrm{d}}{\mathrm{d}t} L \delta t$ and thus the conserved charge is given by

$$H = \frac{\partial L}{\partial \dot{q}} \dot{q} - L \tag{100}$$

which is simply the Hamiltonian (expressed in terms of $(q, \dot{q})$ of the system. So time-translation symmetry implies energy conservation.

(iii) In the first system, we have energy conservation as well as the angular momentum p_φ.
In the second system, p_y is conserved, since the potential does only depend on $x = r\cos\varphi$.

(iv) a) We need the Hamiltonian equation of motions and compute

$$\begin{aligned} \frac{\mathrm{d}O}{\mathrm{d}t} &= \frac{\partial O}{\partial p}\dot{p} + \frac{\partial O}{\partial q}\dot{q} + \frac{\partial O}{\partial t} && (101) \\ &= -\frac{\partial O}{\partial p}\frac{\partial H}{\partial q} + \frac{\partial O}{\partial q}\frac{\partial H}{\partial p} + \frac{\partial O}{\partial t} && (102) \\ &= \{O, H\} + \frac{\partial O}{\partial t}. && (103) \end{aligned}$$

b) We compute

$$\begin{aligned} \frac{\mathrm{d}O}{\mathrm{d}q} &= \frac{\partial O}{\partial q} + \frac{\partial O}{\partial p}\frac{\mathrm{d}p}{\mathrm{d}q} && (104) \\ &= \frac{\partial O}{\partial q}\frac{\mathrm{d}p}{\mathrm{d}p} && (105) \\ &= \{O, p\}. && (106) \end{aligned}$$

c) We compute analogously to above (but the corresponding term in the poisson bracket has the opposite sign)

$$\frac{\mathrm{d}O}{\mathrm{d}p} = -\{O, q\}. \tag{107}$$

(v) We need to perform a Legendre transform relating $\dot{q}$ and p. First we compute $\dot{q}(p, q)$

$$p = \frac{\partial L}{\partial \dot{q}} = \mu\dot{q}^3 - aq \Rightarrow \dot{q} = \left(\frac{1}{\mu}(p + aq)\right)^{\frac{1}{3}}. \tag{108}$$

The Legendre transform is then given by

$$\begin{aligned} H(p,q) &= p\dot{q}(p,q) - L(q, \dot{q}(p,q)) && (109) \\ &= p\left(\frac{1}{\mu}(p+aq)\right)^{\frac{1}{3}} - \frac{\mu}{4}\left(\frac{1}{\mu}(p+aq)\right)^{\frac{4}{3}} - aq\left(\frac{1}{\mu}(p+aq)\right)^{\frac{1}{3}} - \frac{\omega^2}{2}q^2. && (110) \end{aligned}$$

For the second part, we perform another Legendre transform. We first find $p(q, \dot{q})$ to be

$$\dot{q} = \frac{\partial H}{\partial p} = \mu^2 p - \lambda\mu q \Rightarrow p = \frac{1}{\mu^2}(\dot{q} + \lambda\mu q). \tag{111}$$

The Lagrange function is then given by the Legendre transform

$$\begin{aligned} L(q,\dot{q}) &= \dot{q}p(q,\dot{q}) - H(q, p(q,\dot{q})) && (112) \\ &= \dot{q}\frac{1}{\mu^2}(\dot{q} + \lambda\mu q) - \frac{1}{2}\left(\frac{1}{\mu}(\dot{q} + \lambda\mu q) - \lambda q\right)^2. && (113) \\ &= \frac{1}{\mu^2}\dot{q}^2 + \frac{\lambda}{\mu}q\dot{q} - \frac{1}{2\mu^2}\dot{q}^2 && (114) \\ &= \frac{1}{2\mu^2}\dot{q}^2 + \frac{\lambda}{\mu}q\dot{q}. && (115) \end{aligned}$$

(vi) The Hamiltonian is given by

$$H(p,q) = \frac{p^2}{2m} + \frac{\omega^2}{2}q^2. \tag{116}$$

The equations of motion are given by

$$\dot{q} = \frac{p}{m} \tag{117}$$

$$\dot{p} = -m\omega^2 q \tag{118}$$

Inserting one into the other to decouple them gives

$$\ddot{q} = -\frac{m\omega^2}{m}q \tag{119}$$

which is solved e.g. by $q(t) = A\cos(\omega t) + B\sin(\omega t)$. For the momentum, we find

$$p = m\dot{q} = m\omega B\cos(\omega t) - m\omega A\sin(\omega t). \tag{120}$$

Now we only need to impose two initial conditions and we can solve the system. The phase space trajectory is an ellipse. If we have two particles in this potential, we have to figure out a way to draw four-dimensional pictures.