27. Solutions of Hamilton equations of motion as canonical transformations

The state of an N-particle system is described by a point $\xi_i = (p_1, \ldots, p_{3N}, q_1, \ldots, q_{3N})$ in the $6N$-dimensional phase space, with $d^{6N}\xi = d^{3N}p\, d^{3N}q$ as the associated volume element. In this exercise, we will show that the solutions $\xi_i = \xi_i(t, \xi_k^{(0)})$ of Hamilton's equations of motion represent a canonical transformation between the initial point $\xi_k^{(0)} = \xi_k(0)$ and the final point $\xi_i = \xi_i(t)$. In order to be able to carry out the proof stringently, some prior theoretical knowledge is useful, which is to be worked out in the following subtasks.

(a) Matrices, $S \in \mathbb{R}^{(2d)\times(2d)}$ that satisfy the condition

$$S^T J\, S = J \quad \text{mit} \quad J = \begin{pmatrix} 0 & \mathbb{1}_d \\ -\mathbb{1}_d & 0 \end{pmatrix} = -J^T = -J^{-1}$$

are called symplectic. Show that the symplectic matrices form a group in terms of matrix multiplication in which the inverse is given by $S^{-1} = J^T S^T J$. This group is usually abbreviated by $\mathrm{Sp}(d, \mathbb{R})$.

(2 points)

(b) Verify that with the help of the J-matrix the Poisson bracket of two phase space functions $f(p, q)$ and $g(p, q)$

$$\{f, g\}(p, q) = \sum_{i=1}^{3N} \left[\frac{\partial f}{\partial q_i} \frac{\partial g}{\partial p_i} - \frac{\partial g}{\partial q_i} \frac{\partial f}{\partial p_i} \right] ,$$

as well as the Hamilton equations of motion

$$\dot{p}_i = -\frac{\partial H}{\partial q_i} , \quad \dot{q}_i = \frac{\partial H}{\partial p_i}$$

can be rewritten as

$$\{f, g\}(\xi) = -\sum_{i,k=1}^{6N} J_{ik} \frac{\partial f}{\partial \xi_i} \frac{\partial g}{\partial \xi_k} \quad \text{und} \quad \dot{\xi}_i = -\sum_{k=1}^{6N} J_{ik} \frac{\partial H}{\partial \xi_k} .$$

(2 points)

(c) A transformation $\xi_i = \xi_i(\xi_k^{(0)})$ of the phase space points is called canonical if it leaves the Poisson brackets for *all* Phase space functions f and g invariant, i.e. if according to the definition $f(\xi) = f^{(0)}(\xi^{(0)})$

$$\{f, g\}(\xi) = \left\{f^{(0)}, g^{(0)}\right\}(\xi^{(0)}) \quad \forall \quad f, g$$

holds. We now denote the differential of the phase space transformation by the matrix

$$S_{ik}(\xi^{(0)}) = \frac{\partial \xi_i}{\partial \xi_k^{(0)}} = \left(\frac{\partial \xi}{\partial \xi^{(0)}}\right)_{ik} .$$

Show then that:

$$\xi_i = \xi_i(\xi_k^{(0)}) \text{ is canonical} \quad \Longleftrightarrow \quad S^T(\xi^{(0)})\, J\, S(\xi^{(0)}) = J .$$

(4 points)

(d) Let $\xi_i = \xi_i(t, \xi_k^{(0)})$ be the solution of the Hamilton equations of motion

$$\dot{\xi}_i = -\sum_{k=1}^{6N} J_{ik} \frac{\partial H}{\partial \xi_k}$$

for the initial conditions $\xi_k^{(0)}$. Prove that the matrix

$$S_{ik}(t, \xi^{(0)}) = \frac{\partial \xi_i(t, \xi_p^{(0)})}{\partial \xi_k^{(0)}}$$

satisfies the differential equation

$$\frac{dS_{il}}{dt} = -\sum_{j,k=1}^{6N} J_{ij} \left.\frac{\partial^2 H}{\partial \xi_j \partial \xi_k}\right|_{\xi=\xi(\xi^{(0)})} S_{kl}(t, \xi^{(0)})$$

(2 points)

(e) Use this to show that $S_{ik}(t, \xi_p^{(0)})$ is a symplectic matrix for all $t \geq 0$ by considering the derivative of the product $S^T(t, \xi^{(0)})\, J\, S(t, \xi^{(0)})$ after t. Explain why this proves that the transformation $\xi_i = \xi_i(t, \xi_k^{(0)})$ is canonical for all $t \geq 0$?

(3 points)

28. The Liouville equation

Analogous to the last exercise, let $\xi_i = \xi_i(t, \xi_k^{(0)})$ be the solution of the Hamilton equations of motion

$$\dot{\xi}_i = -\sum_{k=1}^{6N} J_{ik} \frac{\partial H}{\partial \xi_k}$$

for the given initial conditions $\xi_k^{(0)}$. Furthermore, let $\Gamma(t)$ describe the phase space region that arises from the temporal evolution of the points of the initial phase space region $\Gamma(0)$.

(a) Using the result $S^T(t, \xi^{(0)})\, J\, S(t, \xi^{(0)}) = J$ from the last exercise, prove Liouville's theorem , which states that the phase space volume over $\Gamma(t)$ is equal to the phase space volume over $\Gamma(0)$, i.e.

$$\int\limits_{\Gamma(t)} d^{6N}\xi = \int\limits_{\Gamma(0)} d^{6N}\xi^{(0)} = \text{const.}$$

(2 points)

Note: From the assumption of constancy of the integral over the phase space density $\rho(t, \xi)$ (total number of „particles“ of an ensemble within $\Gamma(t)$ shall be conserved)

$$\int\limits_{\Gamma(t)} \rho(t, \xi)\, d^{6N}\xi = \int\limits_{\Gamma(0)} \rho(0, \xi^{(0)})\, d^{6N}\xi^{(0)} = \text{const.}$$

follows the Liouville equation

$$\frac{\partial \rho}{\partial t} + \{\rho, H\} = 0$$

as an evolution equation for the phase space density $\rho(t, \xi)$.

29. Probability amplitude for quantum mechanical two-particle scattering (bonus)

In this exercise we want to give a perturbation-theoretic expression for the probability amplitude $w_{\mathrm{f\,i}}$ of the two-particle scattering in a short-range interaction potential $V(|\boldsymbol{x}_1 - \boldsymbol{x}_2|)$. The total Hamiltonian $H = H_0 + V$ includes, in addition to the interaction potential, the Hamiltonian $H_0 = \frac{1}{2m}\left(|\vec{p}_1|^2 + |\vec{p}_2|^2\right)$ of the free time evolution of the two particles. We assume that the initial state of the two particles at time $t_0 = -T$ is the momentum eigenstate $|\psi(-T)\rangle = |\psi_\mathrm{i}\rangle = |\vec{p}_1, \vec{p}_2\rangle$ and are interested in, with which probability the two particles can be found in the impulsion eigenstate $|\psi(T)\rangle = |\psi_\mathrm{f}\rangle = |\vec{p}_1^{\,\prime}, \vec{p}_2^{\,\prime}\rangle$ after the scattering at time $t = T$. Here $H_0|\psi_{\mathrm{i,f}}\rangle = E_{i,f}|\psi_{i,f}\rangle$, where. $E_i = \frac{1}{2m}(|\vec{p}_1|^2 + |\vec{p}_2|^2)$ and $E_f = \frac{1}{2m}(|\vec{p}_1^{\,\prime}|^2 + |\vec{p}_2^{\,\prime}|^2)$ are the associated energy eigenvalues of the free Hamiltonian. Furthermore, let $|\psi_k\rangle$ denote the remaining energy eigenfunctions to H_0 for which the completeness relation $\sum_k |\psi_k\rangle\langle\psi_k| = \mathbb{1}$ holds.

If we denote with $U(t, t_0) = e^{-\frac{i}{\hbar}H(t-t_0)}$ the time evolution operator of the whole dynamics, the probability amplitude of this scattering process is

$$w_{f\,i}(T) = \langle\psi_\mathrm{f}|U(T, -T)|\psi_\mathrm{i}\rangle = \langle\vec{p}_1^{\,\prime}, \vec{p}_2^{\,\prime}|U(T, -T)|\vec{p}_1, \vec{p}_2\rangle\,. \tag{1}$$

In the following we want to determine the two leading terms of this probability amplitude in perturbation theory and show that in the limiting case $T \to \infty$ the energy conservation $E_\mathrm{f} = E_\mathrm{i}$ follows.

(a) First, it makes sense to split off the trivial, free time evolution by considering the problem in the so-called interaction picture. To do this, we define the wave function $|\tilde{\psi}(t)\rangle$ in the interaction picture via $|\psi(t)\rangle = e^{-\frac{i}{\hbar}H_0 t}|\tilde{\psi}(t)\rangle$. Derive from this the Schrödinger equation in the interaction picture

$$i\hbar\frac{\partial}{\partial t}|\tilde{\psi}(t)\rangle = \tilde{V}(t)\,|\tilde{\psi}(t)\rangle, \tag{2}$$

where $\tilde{V}(t) = e^{\frac{i}{\hbar}H_0 t}\,V\,e^{-\frac{i}{\hbar}H_0 t}$.

(1 point)

(b) Verify that $|\tilde{\psi}(t)\rangle = \tilde{U}(t, t_0)|\tilde{\psi}(t_0)\rangle$ with $\tilde{U}(t, t_0) = \mathbb{1} + \sum_{n=1}^{\infty}\tilde{U}^{(n)}(t, t_0)$ and

$$\tilde{U}^{(n)}(t, t_0) = \left(\frac{1}{i\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \ldots \int_{t_0}^{t_{n-1}} dt_n\,\tilde{V}(t_1)\,\tilde{V}(t_2)\ldots\tilde{V}(t_n) \tag{3}$$

are a formal solution of the Schrödinger equation in the interaction picture, Eq. (2) (for arbitrary initial wave functions $|\tilde{\psi}(t_0)\rangle$).

(2 points)

(c) Show that the so-called „diffraction function“

$$\delta_{(\alpha)}(x) = \frac{\sin(\alpha x)}{\pi x}$$

can be written in the form $\delta_{(\alpha)}(x) = \frac{1}{2\pi}\int_{-\alpha}^{\alpha} e^{ix\tau}\,d\tau$ and thus in the limiting case $\alpha \to \infty$ tends towards the δ function.

(1 point)

(d) For short interaction times, it is sufficient to consider the terms $\tilde{U}^{(1)}(t, t_0)$ and $\tilde{U}^{(2)}(t, t_0)$ in the formal solution of the SchrÃ¶dinger equation in the interaction picture and to disregard all higher orders. Under this assumption, using $\langle \psi_\mathrm{f} | \psi_\mathrm{i} \rangle = \delta_\mathrm{fi}$, derive the expression

$$w_{fi}(T) = e^{-\frac{i}{\hbar}(E_\mathrm{f} - E_\mathrm{i})T} \left[\delta_\mathrm{fi} + \langle \psi_\mathrm{f} | \tilde{U}^{(1)}(T, -T) | \psi_\mathrm{i} \rangle + \langle \psi_\mathrm{f} | \tilde{U}^{(2)}(T, -T) | \psi_\mathrm{i} \rangle \right] ,$$

for the probability amplitude (1) and show that

$$\langle \psi_\mathrm{f} | \tilde{U}^{(1)}(T, -T) | \psi_\mathrm{i} \rangle = -2\pi i \, V_\mathrm{fi} \, \delta_{(T/\hbar)}(E_\mathrm{f} - E_\mathrm{i}) ,$$

where we have abbreviated the matrix elements of the interaction potential as $V_{fi} = \langle \psi_\mathrm{f} | V | \psi_\mathrm{i} \rangle$.

(2 points)

(e) Show accordingly for $T \gg 1$ that

$$\langle \psi_\mathrm{f} | \tilde{U}^{(2)}(T, -T) | \psi_\mathrm{i} \rangle \approx -2\pi i \left[\lim_{\varepsilon \to 0+} \sum_k \frac{V_\mathrm{fk} \, V_\mathrm{ki}}{E_\mathrm{i} - E_\mathrm{k} + i\varepsilon} \right] \delta_{(T/\hbar)}(E_\mathrm{f} - E_\mathrm{i})$$

by using the following relation

$$e^{-\frac{i}{\hbar} E_k (t_1 - t_2)} \, \Theta(t_1 - t_2) = -\frac{1}{2\pi i} \lim_{\varepsilon \to 0+} \int_{-\infty}^{\infty} \frac{e^{-\frac{i}{\hbar} E (t_1 - t_2)}}{E - E_k + i\varepsilon} \, dE \, .$$

(3 points)

(f) Finally, we define the transition matrix $\mathcal{T}_\mathrm{f\,i}$ via the relation

$$w_\mathrm{f\,i}(T) = e^{-\frac{i}{\hbar}(E_\mathrm{f} - E_\mathrm{i})T} \left[\delta_\mathrm{fi} - 2\pi i \; \mathcal{T}_\mathrm{f\,i} \, \delta_{(T/\hbar)}(E_\mathrm{f} - E_\mathrm{i}) \right] .$$

Using the above results ($T \gg 1$) and the formal notation,

$$(E \cdot \mathbb{1} - \hat{H}_0 + i\varepsilon \cdot \mathbb{1})^{-1} = \frac{1}{E - H_0 + i\varepsilon}$$

derive the following expression for the transition matrix

$$\mathcal{T}_\mathrm{f\,i} = \lim_{\varepsilon \to 0+} \langle \psi_\mathrm{f} | V + V \, \frac{1}{E_\mathrm{i} - H_0 + i\varepsilon} \, V | \psi_\mathrm{i} \rangle \, .$$

Briefly justify why in the limiting case $T \to \infty$ the conservation of energy $E_\mathrm{f} = E_\mathrm{i}$ is fulfilled.

(2 points)