Lecture 3

12 Change of variables

Basic idea: Map system with unknown solution into a system with known solution.

12.1 Classical mechanics

Action:

$$S(t) := \int_0^t \mathrm{d}\tau \, \left(\frac{m}{2}\, \dot{q}^2 - V(q) \right)$$

Hamilton's characteristic function:

$$W(E) := S(t) + Et = \int_0^t \mathrm{d}\tau \, \left(\frac{m}{2}\, \dot{q}^2 - V(q) + E \right)$$

Change of coordinates: $q \mapsto x \qquad q =: f(x)$

Change of time: $t \mapsto s, \quad \tau \mapsto \sigma$ such that $\mathrm{d}\tau =: g(x)\mathrm{d}\sigma \qquad g$ to be defined

$$\dot{q} = \frac{\mathrm{d}q}{\mathrm{d}\tau} = \frac{f'(x)}{g(x)}\, \mathring{x} \qquad \text{with} \qquad \mathring{(\cdot)} := \frac{\mathrm{d}}{\mathrm{d}\sigma}(\cdot)$$

Consider

$$W(E) = \int_0^t \mathrm{d}\tau \, \left(\frac{m}{2}\, \dot{q}^2 - V(q) + E \right) = \int_0^s \mathrm{d}\sigma \, \left(\frac{m}{2}\, \frac{f'^2(x)}{g(x)}\, \mathring{x}^2 - g(x) \left(V(q) - E \right) \right)$$

Form invariance: $\boxed{f'^2(x) \overset{!}{=} g(x)}$

$$W(E) = \int_0^s \mathrm{d}\sigma \, \left(\frac{m}{2}\, \mathring{x}^2 - \tilde{V}(x) + \tilde{E} \right) =: \tilde{W}(\tilde{E})$$

with

$$\boxed{\begin{array}{rcl} \tilde{V}(x) & := & f'^2(x) \left(V(q) - E \right) + \tilde{V}_0 \\ \tilde{E} & := & \tilde{V}_0 \qquad \text{for convenience, arbitrary} \end{array}}$$

Result: Problem (V, E) in $(q, \tau) \qquad \Longrightarrow \qquad$ Problem $(\tilde{V}, \tilde{E})$ in (x, σ)

Hamilton's characteristic function is invariant under this "form-invariance" transformation.

Example: Radial Kepler problem

$$V(r) = \frac{L^2}{2mr^2} - \frac{\alpha}{r} \qquad \text{with}$$

L: classical angular momentum

α : coupling constant

Let $\quad r = \rho^2 \quad$ that is $\quad f(\rho) = \rho^2\,, \quad g(\rho) = f'^2(\rho) = 4\rho^2\,, \quad \mathrm{d}\tau = 4\rho^2 \mathrm{d}\sigma$

$$\begin{aligned} \tilde{V}(\rho) &= 4\rho^2 \left(\frac{L^2}{2m\rho^4} - \frac{\alpha}{\rho^2} - E \right) + \tilde{V}_0 \\ &= \frac{(2L)^2}{2m\rho^2} - 4E\rho^2 - 4\alpha + \tilde{V}_0 \end{aligned}$$

Choose:

$$\tilde{V}_0 = 4\alpha = \tilde{E}\,, \qquad \tilde{L} = 2L\,, \qquad -4E = \frac{m}{2}\omega^2$$

$$\Longrightarrow \qquad \tilde{V}(\rho) = \frac{\tilde{L}^2}{2m\rho^2} + \frac{m}{2}\omega^2 \rho^2$$

Result:

$$\text{Kepler problem (Newton)} \quad \Longleftrightarrow \quad \text{Harmonic oscillator (Hooke)}$$
$$(L, \alpha, E) \quad \Longleftrightarrow \quad (\tilde{L}, \omega, \tilde{E})$$

Swapping between energy and coupling constants, rescaling of angular momentum

$$4\alpha = \tilde{E}\,, \qquad \omega^2 = -\frac{8E}{m}\,(E < 0 \text{ for bound states})\,, \qquad \tilde{L} = 2L$$

This duality between Kepler and harmonic oscillator was already known to Newton and Hooke.
There exists a more general duality between power-law potentials

$$V(r) = \frac{L^2}{2mr^2} + \lambda_a\, r^a \qquad \text{and} \qquad \tilde{V}(\rho) = \frac{\tilde{L}^2}{2m\rho^2} + \lambda_b\, \rho^b \qquad \text{for} \qquad (a+2)(b+2) = 4.$$

See, e.g., `https://doi.org/10.3390/sym13030409` for details.

12.2 Quantum mechanics

Schrödinger eq. (SE):

$$\left(-\frac{\hbar^2}{2m}\partial_q^2 + V(q) - E\right)\phi(q) = 0$$

Let as before $\quad q =: f(x) \quad$ and now $\quad \phi(q) =: h(x)\varphi(x)$.

Obviously (Homework problem 8): $f'(x) := \partial_x f(x)$ etc.

$$\left(\partial_q^2\right)\phi = \frac{h}{f'^2}\varphi'' + \frac{2h'f' - hf''}{f'^3}\varphi' + \frac{f'h'' - f''h'}{f'^3}\varphi$$

Form invariance: $\boxed{2h'f' = hf''}$ $\quad \varphi'$-term vanishes

$$\Longrightarrow \quad \frac{h'}{h} = \frac{1}{2}\frac{f''}{f'} \quad \Longrightarrow \quad \ln h = \frac{1}{2}\ln f' \quad (+\text{ const} = 0) \quad \Longrightarrow \quad h(x) = \sqrt{f'(x)}$$

Plug into SE:

$$\frac{h}{f'^2}\left(-\frac{\hbar^2}{2m}\varphi'' - \frac{\hbar^2}{2m}\frac{f'h'' - f''h'}{hf'}\varphi\right) + \frac{h}{f'^2}\left(f'^2(V - E)\right)\varphi = 0$$

That is

$$(H - E)\phi = \frac{h}{f'^2}(\tilde{H} - \tilde{E})\varphi = \frac{1}{h^3}(\tilde{H} - \tilde{E})\varphi$$

Noting

$$h' = \frac{1}{2}\frac{f''}{\sqrt{f'}} \qquad \text{and} \qquad h'' = \frac{1}{2f'}\left(\sqrt{f'}f''' - \frac{1}{2}\frac{f''^2}{\sqrt{f'}}\right) = \frac{1}{2}\left(\frac{f'''}{\sqrt{f'}} - \frac{1}{2}\frac{f''^2}{f'^{3/2}}\right)$$

$$\Longrightarrow \qquad \frac{h''}{h} = \frac{1}{2}\frac{f'''}{f'} - \frac{1}{4}\frac{f''^2}{f'^2}$$

$$\Longrightarrow \qquad \frac{h''}{h} - \frac{h'}{h}\frac{f''}{f'} = \frac{1}{2}\frac{f'''}{f'} - \frac{1}{4}\frac{f''^2}{f'^2} - \frac{1}{2}\left(\frac{f''}{f'}\right)^2 = \frac{1}{2}\left(\frac{f'''}{f'} - \frac{3}{2}\frac{f''^2}{f'^2}\right)$$

With Schwarz derivative:

$$(Sf)(x) := \frac{f'''}{f'} - \frac{3}{2}\left(\frac{f''}{f'}\right)^2$$

we arrive at

$$\left[-\frac{\hbar^2}{2m}\left(\partial_x^2+\frac{1}{2}(Sf)(x)\right)+f'^2(x)\left(V(f(x)-E)\right]\varphi(x)=0\,.$$

$\widetilde{\text{SE}}$:

$$\left(\tilde{H}-\tilde{E}\right)\varphi(x):=\left(-\frac{\hbar^2}{2m}\partial_x^2+\tilde{V}(x)-\tilde{E}\right)\varphi(x)=0$$

where

$$\boxed{\begin{array}{rcl}\tilde{V}(x) & := & \underbrace{f'^2(x)\left(V(f(x)-E)+\tilde{V}_0\right.}_{\text{classical part}}-\underbrace{\frac{\hbar^2}{4m}(Sf)(x)}_{\text{quantum part}} \\ \tilde{E} & := & \tilde{V}_0 \qquad \text{for convenience, arbitrary}\end{array}}$$

Result: Problem (V,E_n,ϕ) $\Longrightarrow$ Problem $(\tilde{V},\tilde{E},\varphi)$ with

$$\boxed{\begin{array}{rcl}\phi_n(q) & = & \sqrt{f'(x)}\,\varphi_n(x) \\ E_n & = & \left\{E|\tilde{E}_n(E)=\tilde{V}_0\right\}\end{array}}$$

Remark: φ_n in general not normalized as

$$\int \mathrm{d}q\,\phi_n^2(q)=\int \mathrm{d}x\,f'(x)f'(x)\varphi_n^2(x)$$

Example: Coulomb problem

$$V(r)=\frac{\hbar^2\ell(\ell+1)}{2mr^2}-\frac{\alpha}{r}$$

Again we let $r=\rho^2=f(\rho)\,,\quad\to\quad f'=2\rho\,,\quad f''=2\,,\quad f'''=0\,.$

Schwarz derivative: $(Sf)(\rho)=-\frac{3}{2}\left(\frac{2}{2\rho}\right)^2=-\frac{3}{2\rho^2}$

New eff. potential:

$$\begin{aligned}\tilde{V}(\rho)&=4\rho^2\left(\frac{\hbar^2\ell(\ell+1)}{2m\rho^4}-\frac{\alpha}{\rho^2}-E\right)+\tilde{V}_0-\frac{\hbar^2}{4m}\left(-\frac{3}{2\rho^2}\right)\\&=\frac{\hbar^2}{2m\rho^2}\left(4\ell^2+4\ell+\frac{3}{4}\right)-4\alpha-4E\rho^2+\tilde{V}_0\end{aligned}$$

When we let $\tilde{\ell}+\frac{1}{2}:=2(\ell+\frac{1}{2})\quad\to\quad\tilde{\ell}=2\ell+\frac{1}{2}\quad\to\quad\tilde{\ell}(\tilde{\ell}+1)=4\ell^2+4\ell+\frac{3}{4}$
we arrive at the harmonic oscillator problem

$$\tilde{V}(\rho)=\frac{\hbar^2}{2m\rho^2}\tilde{\ell}(\tilde{\ell}+1)+\frac{m}{2}\omega^2\rho^2$$

with $\tilde{\ell}=2\ell+\frac{1}{2}\,,\quad\tilde{V}_0=\tilde{E}=4\alpha\,,\quad\omega^2=-\frac{8E}{m}$

In QM the Coulomb and harmonic oscillator (HO) problem are quasi-dual to each other.

Quasi-dual because an integer $\ell\in\mathbb{N}_0$ results in half-odd integers $\tilde{\ell}$.

However, both are simply parameters in the radial SE and hence this is not really a restriction. We treat them as real numbers and only in the end we may imply the angular momentum quantisation.

Comment:
It is known that the WKB approximation provides the exact spectrum for the 1-dim. HO but not for the radial HO or Coulomb problem. Only upon the ad-hoc Langer modification, where the replacement $\ell(\ell+1)\to(\ell+\frac{1}{2})^2$ is imposed. Recall the classical relation $\tilde{L}^2=4L^2$

and impose Langer modification on both sides $(\tilde{\ell}+\frac{1}{2})^2 = 4(\ell+\frac{1}{2})^2$. This is precisely the exact relation $\tilde{\ell} = 2\ell + \frac{1}{2}$ found above. See Homework problem 9.

Energy eigenvalues:
We know the spectrum for the radial HO

$$\tilde{E}_{n\tilde{\ell}}(E) = \hbar\omega\left(2n + \tilde{\ell} + \frac{3}{2}\right) = \hbar\omega(2n + 2\ell + 2) \stackrel{!}{=} \tilde{V}_0 = 4\alpha$$

$$\Longrightarrow \quad \omega^2 = \left(\frac{4\alpha}{\hbar}\right)^2 \frac{1}{(2n+2\ell+2)^2} \stackrel{!}{=} -\frac{8E_{n\ell}}{m}$$

$$\Longrightarrow \quad E_{n\ell} = -\frac{m\alpha^2}{2\hbar^2}\frac{1}{(n+\ell+1)^2} \qquad \text{Coulomb specrum!!!}$$

Remarks:

- For the energy eigenfunctions see tutorial exercise 9
- The quantum case is almost identical to the classical case
- change of time in classical system $\Longleftrightarrow$ change of wave function in QM.
  Recall also the classical time transformation $\partial_\tau = \frac{1}{g}\partial_\sigma = \frac{1}{f'^2}\partial_\sigma$. This transforms into

$$(\mathrm{i}\hbar\partial_\tau - H)\phi = \frac{h}{f'^2}(\mathrm{i}\hbar\partial_\sigma - \tilde{H})\varphi = 0 \qquad \text{with} \qquad \phi(q,\tau) = h(x)\varphi(x,\sigma)$$

- How does this show up in path integrals?

12.3 Change of variables in path integrals

Recall Green's function and promotor

$$\begin{aligned} G(\vec{x}'',\vec{x}';E) := \langle\vec{x}''|\frac{1}{H-E}|\vec{x}'\rangle \quad &= \frac{\mathrm{i}}{\hbar}\int_0^\infty \mathrm{d}t\,\langle\vec{x}''|\mathrm{e}^{-(\mathrm{i}/\hbar)(H-E)t}|\vec{x}'\rangle \\ &= \frac{\mathrm{i}}{\hbar}\int_0^\infty \mathrm{d}t\,P_E(x'',x';t) \end{aligned}$$

with promotor

$$P_E(x'',x';t) := \langle x''|\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}(\hat{H}-E)t}|x'\rangle$$

Let's look at the spectral representation (for simplicity purely discrete spectrum)

$$G(q'',q';E) = \sum_n \frac{\phi(q'')\phi^*(q')}{E-E_n} \stackrel{?}{=} \sqrt{f'(x'')f'(x')}\sum_n \frac{\varphi(x'')\varphi^*(x')}{\tilde{E}-\tilde{E}_n(E)} = h(x'')h(x')\tilde{G}(x'',x';\tilde{E})$$

Proof: Recall relation $\quad (H-E)_q\,h(x) = \frac{1}{h^3(x)}(\tilde{H}-\tilde{E})_x \quad$ with $\quad h(x) = \sqrt{f'(x)}$
and $\quad (H-E)_q\,G(q,q';E) = \delta(q-q') \quad \Longrightarrow$

$$\delta(q-q') = (H-E)_q\,h(x)h(x')\tilde{G}(x,x';\tilde{E}) = \frac{h(x')}{h^3(x)}(\tilde{H}-\tilde{E})_x\,\tilde{G}(x,x';\tilde{E}) = \frac{h(x')}{h^3(x)}\delta(x-x') = \frac{1}{f'(x)}\delta(x-x')$$

This is correct as $q = f(x)$.

Implies a relation for the integrated promotors:

$$\begin{aligned} G(q'',q';E) \quad &= \frac{\mathrm{i}}{\hbar}\int_0^\infty \mathrm{d}t\,P_E(q'',q';t) \\ &= \sqrt{f'(x'')f'(x')}\tilde{G}(x'',x';\tilde{E}) = \frac{\mathrm{i}}{\hbar}\sqrt{f'(x'')f'(x')}\int_0^\infty \mathrm{d}s\,\tilde{P}_{\tilde{E}}(x'',x';s) \end{aligned}$$

Both promotors exhibit a path integral representation

$$P_E(q'',q';t)=\int_{q'=q(0)}^{q''=q(t)}\mathcal{D}[q(\tau)]\exp\left\{\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}\tau\left(\frac{m}{2}\dot{q}^2-V(q)+E\right)\right\}$$

$$\tilde{P}_{\tilde{E}}(x'',x';s)=\int_{x'=x(0)}^{x''=x(t)}\mathcal{D}[x(\sigma)]\exp\left\{\frac{\mathrm{i}}{\hbar}\int_0^s \mathrm{d}\sigma\left(\frac{m}{2}\dot{x}^2-\tilde{V}(x)+\tilde{E}\right)\right\}$$

They are related via the point transformation $q=f(x)$.

Questions:

- How shall we implement the classical relation $\mathrm{d}\tau=f'^2(x)\mathrm{d}\sigma$?
  A priory, the parameters t and s are independent in above derivation.
- How are the potentials and energies related?
  Can we recover the same relations as in the classical case and/or for the SE?

Point transformation in time-sliced path integrals
We start with $P_E(q'',q';t)$ and hope to arrive more or less at $\tilde{P}_{\tilde{E}}(x'',x';s)$.

$$P_E(q'',q';t)=\lim_{N\to\infty}\prod_{j=1}^{N-1}\int\mathrm{d}q_j\prod_{j=1}^{N}\left(\frac{m}{2\pi\mathrm{i}\hbar\varepsilon}\right)^{1/2}\mathrm{e}^{(\mathrm{i}/\hbar)W_j(E)}$$

with

$$W_j(E)=\frac{m}{2}\frac{(\Delta q_j)^2}{\varepsilon}-V(q_j)\varepsilon+E\varepsilon$$

The point transformation $q=f(x)$ implies: $\Delta q_j=q_j-q_{j-1}=f(x_j)-f(x_{j-1})=:f_j-f_{j-1}$

Tutorial Exercise 8: $(\Delta q_j)^2=f'_jf'_{j-1}(\Delta x_j)^2+\left(\frac{1}{4}f''^2_j-\frac{1}{6}f'''_jf'_j\right)(\Delta x_j)^4+O((\Delta x_j)^6)$
Recall the rule

$$\int\mathrm{d}x\,\mathrm{e}^{-\frac{a}{\sigma}x^2+\frac{b}{\sigma}x^4}=\int\mathrm{d}x\,\mathrm{e}^{-\frac{a}{\sigma}x^2+\frac{3b}{4a^2}\sigma+O(\sigma^2)}$$

With

$$\frac{\mathrm{i}m}{2\hbar\varepsilon}(\Delta q_j)^2=\frac{\mathrm{i}mf'_jf''_{j-1}}{2\hbar\varepsilon}(\Delta x_j)^2+\frac{\mathrm{i}mf'_jf''_{j-1}}{2\hbar\varepsilon}\left(\frac{1}{4}f''^2_j-\frac{1}{6}f'''_jf'_j\right)(\Delta x_j)^4\frac{1}{f'_jf''_{j-1}}$$

we have

$$\sigma=\frac{\varepsilon}{f'_jf''_{j-1}},\quad a=\frac{m}{2\mathrm{i}\hbar},\quad b=\frac{\mathrm{i}m}{2\hbar}\left(\frac{1}{4}\frac{f''^2_j}{f'^2}-\frac{1}{6}\frac{f'''_jf'_j}{f'_j}\right)=-\frac{\mathrm{i}m}{12\hbar}\left(\frac{f'''_j}{f'_j}-\frac{3}{2}\frac{f''^2_j}{f'^2_j}\right)=-\frac{\mathrm{i}m}{12\hbar}(Sf)(x_j)$$

Hence we may approximate the higher order term as follows

$$\frac{\mathrm{i}m}{2\hbar\varepsilon}(\Delta q_j)^2\approx\frac{\mathrm{i}m}{2\hbar\sigma}(\Delta x_j)^2+\frac{3}{4}\left(\frac{2\mathrm{i}\hbar}{m}\right)^2\left(-\frac{\mathrm{i}m}{12\hbar}\right)(Sf)(x_j)\sigma=\frac{\mathrm{i}}{\hbar}\left(\frac{m}{2\sigma}(\Delta x_j)^2+\frac{\hbar^2}{4m}(Sf)(x_j)\sigma\right)$$

$\Longrightarrow$

$$W_j(E)=\frac{m}{2\sigma}(\Delta x_j)^2-\tilde{V}(x_j)\sigma+\tilde{E}\sigma$$

where

$$\tilde{V}(x)=f'^2(x)\left(V(f(x))-E\right)+\tilde{V}_0-\frac{\hbar^2}{4m}(Sf)(x_j)\,,\qquad\tilde{E}=\tilde{V}_0$$

We arrive at the same result as via SE.

Looking at the measure

$$\prod_{j=1}^{N-1} \mathrm{d}q_j \prod_{j=1}^{N} \sqrt{\frac{m}{2\pi\mathrm{i}\hbar\varepsilon}} = \prod_{j=1}^{N-1} \mathrm{d}x_j\, f'_j \prod_{j=1}^{N} \left(\frac{m}{2\pi\mathrm{i}\hbar\sigma f'_j f'_{j-1}}\right)^{1/2}$$
$$= \frac{1}{\sqrt{f'(x'')f'(x')}} \prod_{j=1}^{N-1} \mathrm{d}x_j \prod_{j=1}^{N} \left(\frac{m}{2\pi\mathrm{i}\hbar\sigma}\right)^{1/2}$$

Result

$$P_E(q'',q';t) = \frac{1}{\sqrt{f'(x'')f'(x')}} \underbrace{\lim_{N\to\infty} \prod_{j=1}^{N-1} \int \mathrm{d}x_j \prod_{j=1}^{N} \left(\frac{m}{2\pi\mathrm{i}\hbar\sigma}\right)^{1/2} \mathrm{e}^{(\mathrm{i}/\hbar)\tilde{W}_j(\tilde{E})}}_{=\tilde{P}_{\tilde{E}}(x'',x';s) \quad s=N\sigma}$$

Compare with previous result

$$G(q'',q';E) = \frac{\mathrm{i}}{\hbar}\int_0^\infty \mathrm{d}t\, P_E(q'',q';t)$$
$$= \frac{\mathrm{i}}{\hbar}\int_0^\infty \mathrm{d}t\, \frac{1}{\sqrt{f'(x'')f'(x')}} \tilde{P}_{\tilde{E}}(x'',x';s)$$
$$\stackrel{!}{=} \frac{\mathrm{i}}{\hbar}\sqrt{f'(x'')f'(x')} \int_0^\infty \mathrm{d}s\, \tilde{P}_{\tilde{E}}(x'',x';s)$$

Obviously we cannot do the t-integral in the second line as we have no relation between t and s.
However, the last line suggests the formal substitution

$$\text{"}\mathrm{d}t = f'(x'')f'(x')\,\mathrm{d}s\text{"}\,.$$

In essence, we can reproduce the result of the SE also within the path integral. However, one needs to consider the Green's function and the integrated promotors represented by a path integral.

13 Path integration for the Coulomb problem

Here we will apply the above change of variables to the Coulomb problem represented by potential

$$V(r) = -\frac{\alpha}{r}\,, \qquad r = |\vec{r}|\,.$$

13.1 Propagator and angular integration

Obviously the propagator is given via below path integral representation

$$K(\vec{r}'',\vec{r}';t) = \int_{\vec{r}'=\vec{r}(0)}^{\vec{r}''=\vec{r}(t)} \mathcal{D}[\vec{r}(\tau)] \exp\left\{\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}\tau \left(\frac{m}{2}\dot{\vec{r}}^2 + \frac{\alpha}{r}\right)\right\}$$
$$= \lim_{N\to\infty} \prod_{j=1}^{N-1} \int \mathrm{d}^3\vec{r}_j \prod_{j=1}^{N} \left(\frac{m}{2\pi\mathrm{i}\hbar\varepsilon}\right)^{3/2} \mathrm{e}^{(\mathrm{i}/\hbar)S_j}$$
$$\text{with} \quad S_j = \frac{m}{2\varepsilon}(\Delta\vec{r}_j)^2 + \frac{\alpha}{r_j}\varepsilon$$

We note that due to it spherical symmetry we can apply the decomposition in polar coordinates as discussed in section 10 to arrive at

$$K(\vec{r}'',\vec{r}';t)=\sum_{\ell=0}^{\infty}K_\ell(r'',r';t)\sum_{\mu=-\ell}^{\ell}Y_{\ell\mu}(\theta'',\varphi'')Y^*_{\ell\mu}(\theta',\varphi')$$

with radial path integral

$$K_\ell(r'',r';t):=\lim_{N\to\infty}\prod_{j=1}^{N-1}\int_0^\infty \mathrm{d}r_j\, r_j^2\prod_{j=1}^{N}k_\ell(r_j,r_{j-1};\varepsilon)$$

where (recall $\hat{r}_j^2=r_jr_{j-1}$)

$$k_\ell(r_j,r_{j-1};\varepsilon)=\frac{m}{\mathrm{i}\hbar\varepsilon\sqrt{r_jr_{j-1}}}\exp\left\{\frac{\mathrm{i}}{\hbar}\left[\frac{m}{2\varepsilon}(r_j^2+r_{j-1}^2)+\frac{\alpha}{\hat{r}_j}\varepsilon\right]\right\}\mathrm{I}_{\ell+\frac{1}{2}}\left(\frac{m\hat{r}_j^2}{\mathrm{i}\hbar\varepsilon}\right).$$

13.2 The radial Green's function

Similar to the propagator, the Green's function decomposes into a radial and angular part

$$G(\vec{r}'',\vec{r}';E)=\sum_{\ell=0}^{\infty}G_\ell(r'',r';E)\sum_{\mu=-\ell}^{\ell}Y_{\ell\mu}(\theta'',\varphi'')Y^*_{\ell\mu}(\theta',\varphi')$$

with radial Green's function given by

$$G_\ell(r'',r';E)=\frac{\mathrm{i}}{\hbar}\int_0^\infty \mathrm{d}t\, K_\ell(r'',r';t)\,\mathrm{e}^{(\mathrm{i}/\hbar)Et}=\frac{\mathrm{i}}{\hbar}\int_0^\infty \mathrm{d}t\, P_{E\ell}(r'',r';t)$$

Here the radial promotor is expressed by the formal radial path integral

$$P_{E\ell}(r'',r';t)=\int_{r'=r(0)}^{r''=r(t)}\mathcal{D}[r(\tau)]\exp\left\{\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}\tau\left(\frac{m}{2}\dot{r}^2-\frac{\ell(\ell+1)\hbar^2}{2mr^2}+\frac{\alpha}{r}+E\right)\right\}$$

Now we perform the point transformation $r=\rho^2$, that is, $f(\rho)=\rho^2$. This implies

$$f'(\rho)=2\rho\,,\qquad \mathrm{d}\tau=4\rho^2\mathrm{d}\sigma\qquad\text{or}\qquad \varepsilon=4\rho_j\rho_{j-1}\sigma$$

The new effective potential is given by (cf. example in section 11.2)

$$\tilde{V}(\rho)=\frac{\hbar^2}{2m\rho^2}\tilde{\ell}(\tilde{\ell}+1)+\frac{m}{2}\omega^2\rho^2$$

with $\quad\tilde{\ell}=2\ell+\frac{1}{2}\,,\quad \tilde{E}=4\alpha\,,\quad \omega^2=-\frac{8E}{m}$

Hence we arrive at

$$G_\ell(r'',r';E)=\frac{\mathrm{i}}{\hbar}\sqrt{4\rho''\rho'}\int_0^\infty \mathrm{d}s\,\tilde{P}_{\tilde{E}\tilde{\ell}}(\rho'',\rho';s)$$

with

$$\tilde{P}_{\tilde{E}\tilde{\ell}}(\rho'',\rho';s)=\int_{\rho'=\rho(0)}^{\rho''=x(t)}\mathcal{D}[\rho(\sigma)]\exp\left\{\frac{\mathrm{i}}{\hbar}\int_0^s \mathrm{d}\sigma\left(\frac{m}{2}\mathring{\rho}^2-\tilde{V}(\rho)+\tilde{E}\right)\right\}$$

and

$$\tilde{V}(\rho)=\frac{\tilde{\ell}(\tilde{\ell}+1)\hbar^2}{2m\rho^2}+\frac{m}{2}\omega^2\rho^2\,,$$

which is the radial harmonic oscillator path integral plus a constant $\tilde{E} = 4\alpha$.
This we already solved in section 10.3 with the result

$$\tilde{P}_{\tilde{E}\tilde{\ell}}(\rho'', \rho'; s) = \frac{1}{\sqrt{\rho''\rho'}} \frac{m\omega}{\mathrm{i}\hbar \sin\omega s} \exp\left\{\frac{\mathrm{i}}{\hbar}\frac{m\omega}{2}({\rho''}^2 + {\rho'}^2)\cot\omega s\right\} \mathrm{I}_{\tilde{\ell}+\frac{1}{2}}\left(\frac{m\omega\rho''\rho'}{\mathrm{i}\hbar\sin\omega s}\right) \mathrm{e}^{(\mathrm{i}/\hbar)4\alpha s}$$

The remaining s integration can explicitly be performed resulting in

$$\begin{aligned} G_\ell(r'', r'; E) &= \frac{\mathrm{i}}{\hbar}\sqrt{4\rho''\rho'}\int_0^\infty \mathrm{d}s\, \tilde{P}_{\tilde{E}\tilde{\ell}}(\rho'', \rho'; s) \\ &= \frac{\mathrm{i}m}{kr''r'\hbar^2}\frac{\Gamma(\ell - \mathrm{i}\nu + 1)}{\Gamma(2\ell+2)} W_{\mathrm{i}\nu,\ell+\frac{1}{2}}(-2\mathrm{i}kr_+) M_{\mathrm{i}\nu,\ell+\frac{1}{2}}(-2\mathrm{i}kr_-) \end{aligned}$$

Here W and M are the linearly independent Whittaker functions (confluent hypergeometric function) and we have set

$$r_+ = \max(r'', r')\,, \quad r_- = \min(r'', r')\,, \quad \alpha = \frac{\hbar^2 k\nu}{m}\,, \quad E = \frac{\hbar^2 k^2}{2m}\,.$$

Note that $\operatorname{Im} E > 0 \Leftrightarrow \operatorname{Im} k > 0$ and $m\omega = -2\mathrm{i}\hbar k$ and $\tilde{E} = 4\alpha \Rightarrow \mathrm{i}\nu = \tilde{E}/2\hbar\omega$.
For the experts, use below formula with $q = \mathrm{i}\omega s$ and $\mu = \ell + \frac{1}{2}$ for $a > b$

$$\int_0^\infty \mathrm{d}q\, \frac{1}{\sinh q}\,\mathrm{e}^{-\frac{1}{2}(a+b)t\coth q}\,\mathrm{e}^{2\nu q}\,\mathrm{I}_{2\mu}\left(\frac{t\sqrt{ab}}{\sinh q}\right) = \frac{\Gamma(\frac{1}{2}+\mu-\nu)}{t\sqrt{ab}\Gamma(2\mu+1)} W_{\nu,\mu}(at) M_{\nu,\mu}(bt)$$

Homework: Derive the Coulomb spectrum from the poles of $G_\ell(r'', r'; E)$.
For more general duality relations see: `https://doi.org/10.1088/1751-8121/ad213d`

14 Particle confined on a ring

Consider a particle of mass $m > 0$ moving around a ring S^1 of radius $R > 0$.

Hilbert space: $\mathcal{H} := L^2(S^1)\,, \qquad S^1 = \{\varphi | 0 \le \varphi < 2\pi\}$

Hamiltonian: $H = \frac{L_z^2}{2m} = -\frac{\hbar^2}{2mR^2}\frac{\partial^2}{\partial\varphi^2}$

Eigenfunctions: $\psi(\varphi) = \frac{1}{\sqrt{2\pi}}\mathrm{e}^{\mathrm{i}\ell\varphi} = \psi(\varphi + 2\pi)\,, \qquad \ell \in \mathbb{Z}$

Eigenvalues: $E_\ell = \frac{\hbar^2\ell^2}{2mR^2}$

Propagator:
Use spectral representation (also called angular momentum representation)

$$K(\varphi'', \varphi', t) = \sum_{\ell=-\infty}^{\infty}\frac{1}{2\pi}\exp\left\{-\frac{\mathrm{i}}{\hbar}\frac{\hbar^2\ell^2}{2mR^2}t\right\}\mathrm{e}^{\mathrm{i}\ell(\varphi''-\varphi')}$$

Jacobi's Theta function: See Homework 3 Problem 11

$$\Theta(z|\tau) := \sum_{\ell\in\mathbb{Z}}\exp\left\{\mathrm{i}\pi\ell^2\tau + 2\pi\mathrm{i}\ell z\right\}\,, \qquad z \in \mathbb{C}\,, \qquad \operatorname{Im}\tau > 0\,.$$

Let $z := \frac{\varphi'' - \varphi'}{2\pi}\,, \qquad \pi\tau := -\frac{\hbar t}{2mR^2}$ recall $\operatorname{Im} m > 0$

$$\Longrightarrow \qquad K(\varphi'', \varphi', t) = \frac{1}{2\pi}\Theta\left(\frac{\varphi''-\varphi'}{2\pi}\,\middle|\, -\frac{\hbar t}{2mR^2}\right)$$

From homework:

$$\Theta(z|\tau) = \sqrt{\frac{\mathrm{i}}{\tau}}\,\mathrm{e}^{-\mathrm{i}\pi z^2/\tau}\,\Theta\left(\frac{z}{\tau}\middle|-\frac{1}{\tau}\right)$$

Propagator:

$$\begin{aligned}K(\varphi'',\varphi',t) &= \frac{1}{2\pi}\sqrt{\frac{2mR^2\pi\mathrm{i}}{-\hbar t}}\exp\left\{-\mathrm{i}\pi\left(\frac{\varphi''-\varphi'}{2\pi}\right)^2\left(\frac{2mR^2\pi}{-\hbar t}\right)\right\}\Theta\left(\frac{z}{\tau}\middle|-\frac{1}{\tau}\right)\\ &= \sqrt{\frac{mR^2}{2\pi\mathrm{i}\hbar t}}\exp\left\{\frac{\mathrm{i}}{\hbar}\frac{mR^2}{2t}(\varphi''-\varphi')^2\right\}\sum_{n\in\mathbb{Z}}\exp\left\{-\mathrm{i}\pi\frac{n^2}{\tau}+2\pi\mathrm{i}\frac{nz}{\tau}\right\}\end{aligned}$$

Let us look into the exponent in more detail

$$\begin{aligned}&\frac{\mathrm{i}}{\hbar}\frac{mR^2}{2t}(\varphi''-\varphi')^2+\mathrm{i}\pi n^2\frac{2mR^2\pi}{\hbar t}+2\pi\mathrm{i}n\frac{\varphi''-\varphi'}{2\pi}\frac{2mR^2\pi}{-\hbar t}\\ &\quad=\frac{\mathrm{i}}{\hbar}\frac{mR^2}{2t}\left[(\varphi''-\varphi')^2-2n(\varphi''-\varphi')2\pi+4\pi^2n^2\right]\\ &\quad=\frac{\mathrm{i}}{\hbar}\frac{mR^2}{2t}\left(\varphi''-\varphi'-2\pi n\right)^2\end{aligned}$$

Propagator in winding number representation

$$\begin{aligned}K(\varphi'',\varphi',t) &= \sqrt{\frac{mR^2}{2\pi\mathrm{i}\hbar t}}\sum_{n\in\mathbb{Z}}\exp\left\{\frac{\mathrm{i}}{\hbar}\frac{mR^2}{2t}(\varphi''-\varphi'+2\pi n)^2\right\}\\ &= \sum_{n\in\mathbb{Z}}K_n(\varphi'',\varphi',t)\end{aligned}$$

with

$$K_n(\varphi'',\varphi',t) := \sqrt{\frac{mR^2}{2\pi\mathrm{i}\hbar t}}\exp\left\{\frac{\mathrm{i}}{\hbar}\frac{mR^2}{2t}(\varphi''-\varphi'+2\pi n)^2\right\}$$

Distance $x''-x'$ between initial and final point

$$x''-x' = R(\varphi''-\varphi'+2\pi n) \qquad \text{with } n \text{ full cycles}$$

Like free particle on line with $\mathrm{d}x = R\mathrm{d}\varphi$

$$K_n(\varphi'',\varphi',t) := R\sqrt{\frac{m}{2\pi\mathrm{i}\hbar t}}\exp\left\{\frac{\mathrm{i}}{\hbar}\frac{m}{2t}(x''-x')^2\right\}$$

Remarks:

- S^1 is multiple connected space
- Winding number n classifies all paths within one homotopic class
- Paths belonging to different homotopic class cannot be deformed into each other
- K_n is partial propagator for homotypic class n

Laidlaw/DeWitt (1971) and Dowker (1972):
Propagator on multiple connected space $\mathcal{M}$

$$K(x'',x';t) = \sum_{\alpha}\chi(\alpha)\,K_\alpha(x'',x',t)$$

α: Represents homotopy class of paths from x' to x''
$\chi(\alpha)$: Unitarity representation of fundamental homotopy group of $\mathcal{M}$, $\pi_1(\mathcal{M})$

Our example: $S^1 = \mathbb{R}/\mathbb{Z}$
$\mathbb{R}$: Universal covering space
$\mathbb{Z}$: Fundamental group
Unitary reps.: $\chi^{(\delta)}(n) = \mathrm{e}^{-\mathrm{i}\delta n}$ $\quad \delta \in [0, 2\pi[$ $\quad$ arbitrary
Our derivation resulted in trivial reps. $\delta = 0$ where $\chi^{(0)}(n) = 1$.

Using a non-trivial reps.: $\delta \neq 0$

Let

$$\begin{aligned} K^{\delta}(\varphi'', \varphi', t) &:= \sum_{n\in\mathbb{Z}} \mathrm{e}^{-\mathrm{i}\delta n}\, K_n(\varphi'', \varphi', t) \\ &= \sum_{n\in\mathbb{Z}} \mathrm{e}^{-\mathrm{i}\delta n} \sqrt{\frac{mR^2}{2\pi \mathrm{i}\hbar t}} \exp\left\{ \frac{\mathrm{i}}{\hbar} \frac{mR^2}{2t} (\varphi'' - \varphi' + 2\pi n)^2 \right\} \\ &\qquad \cdots \qquad \text{Tutorial Excercise 11} \qquad \cdots \\ &= \sum_{\ell\in\mathbb{Z}} \frac{1}{2\pi} \exp\left\{ -\frac{\mathrm{i}}{\hbar} \frac{\hbar^2 \left(\ell - \frac{\delta}{2\pi}\right)^2}{2mR^2} t \right\} \mathrm{e}^{\mathrm{i}\left(\ell - \frac{\delta}{2\pi}\right)(\varphi'' - \varphi')} \end{aligned}$$

That is, the spectral properties now read

$$E_\ell = \frac{\hbar^2}{2mR^2} \left(\ell - \frac{\delta}{2\pi} \right)^2 , \qquad \psi_\ell(\varphi) = \frac{1}{\sqrt{2\pi}} \exp\left\{ \mathrm{i} \left(\ell - \frac{\delta}{2\pi} \right) \varphi \right\}$$

They still obey the same Schrödinger eq.

$$-\frac{\hbar^2}{2mR^2} \frac{\partial^2}{\partial \varphi^2} \psi_\ell(\varphi) = E_\ell \, \psi_\ell(\varphi) \, .$$

So what is the physical meaning of δ? $\Longrightarrow$ AB-effect