3.2. Hamiltonians Quadratic in Momentum Variables

The Consistency

Consider a hamiltonian

$$H = \frac{p^2}{2m} + V(q)$$

that gives rise to a classical action [see eq(3.8)],

$$S(p, q) = -\int_{t'}^{t''} dt\, L = \int_{t'}^{t''} dt\,(-i\,p\,\dot{q} + H)$$

$$= \int_{t'}^{t''} dt\left(-i\,p\,\dot{q} + \frac{p^2}{2m} + V\right) \tag{3.10}$$

On the classical path

$$p = i\,m\,\dot{q}$$

Following §2.5.1, we thus set

$$p(t) = i\,m\,\dot{q}(t) + r(t) \tag{3.11}$$

so that

$$-L = -i\,(i\,m\,\dot{q} + r)\,\dot{q} + \frac{1}{2m}(i\,m\,\dot{q} + r)^2 + V$$

$$= \frac{1}{2m}r^2 + \frac{1}{2}m\,\dot{q}^2 + V$$

$$\to \qquad S = \int_{t'}^{t''} dt\left(\frac{1}{2m}r^2 + \frac{1}{2}m\,\dot{q}^2 + V\right)$$

With

$$d\,p = d\,r$$

eq(3.9) becomes

$$\langle q'' \mid U(t'', t') \mid q' \rangle = \lim_{n\to\infty} \int \prod_{j=1}^{n} \frac{d\,r_j}{2\pi\hbar} \exp\left(-\frac{1}{\hbar}\int_{t'}^{t''} dt\,\frac{1}{2m}r^2\right)$$

$$\times \int \prod_{k=1}^{n-1} d\,q_k \exp\left[-\frac{1}{\hbar}\int_{t'}^{t''} dt\left(\frac{1}{2}m\,\dot{q}^2 + V\right)\right]$$

Using

$$\int_{-\infty}^{\infty} \frac{d\,r}{2\pi\hbar} \exp\left(-\frac{r^2}{2m\hbar}\right) = \sqrt{\frac{m}{2\pi\hbar}}$$

we have

$$\langle q'' \mid U(t'', t') \mid q' \rangle = \lim_{n\to\infty} \left(\frac{m}{2\pi\hbar}\right)^{n/2} \int \prod_{k=1}^{n-1} d\,q_k \exp\left[-\frac{1}{\hbar}\int_{t'}^{t''} dt\left(\frac{1}{2}m\,\dot{q}^2 + V\right)\right]$$

$$= \int_{q(t')=q'}^{q(t'')=q''} [d\,q(t)] \exp\left[-\frac{1}{\hbar}\int_{t'}^{t''} dt\left(\frac{1}{2}m\,\dot{q}^2 + V\right)\right] \tag{3.12}$$

which is exactly eq(2.19).

Particle in a Magnetic Field

Consider the classical hamiltonian

$$H = \frac{(\boldsymbol{p} - e\,\boldsymbol{A})^2}{2\,m} + V(\boldsymbol{q}) \tag{3.13}$$

where $\boldsymbol{A}$ is the vector potential & e is the electric charge.

Note that our e is the negative of that used by Zinn-Justin.

H is gauge invariant, i.e., under the transformation

$$\boldsymbol{A} \;\to\; \boldsymbol{A}' = \boldsymbol{A} + \nabla\Lambda \qquad (\,\Lambda \text{ arbitary}\,)$$

The eq. of motion (real time) for eq(3.13) is

$$\dot{p}_i = -\partial_i H = \frac{e}{m}(\boldsymbol{p} - e\,\boldsymbol{A})\cdot\partial_i \boldsymbol{A} - \partial_i V \qquad \left(\,\partial_i = \frac{\partial}{\partial\, q_i}\,\right)$$

$$= e\,\boldsymbol{v}\cdot\partial_i \boldsymbol{A} - \partial_i V \qquad \left[\,\boldsymbol{v} = \dot{\boldsymbol{q}} = \frac{1}{m}(\boldsymbol{p} - e\,\boldsymbol{A})\,\right]$$

Using

$$(\boldsymbol{v}\times\boldsymbol{B})_i = \epsilon_{ijk}\, v_j\, B_k \;= \epsilon_{ijk}\,\epsilon_{klm}\, v_j\, \partial_l A_m \;= \left(\delta_{il}\,\delta_{jm} - \delta_{im}\,\delta_{jl}\right) v_j\, \partial_l A_m$$

$$= v_j\left(\partial_i A_j - \partial_j A_i\right) = \boldsymbol{v}\cdot\partial_i \boldsymbol{A} - (\boldsymbol{v}\cdot\nabla)\, A_i$$

$$= \boldsymbol{v}\cdot\partial_i \boldsymbol{A} - \frac{d\,A_i}{d\,t} + \frac{\partial\,A_i}{\partial\,t}$$

$$= \boldsymbol{v}\cdot\partial_i \boldsymbol{A} - \frac{d\,A_i}{d\,t} \qquad \text{if} \qquad \boldsymbol{A} = \boldsymbol{A}(\boldsymbol{q})$$

we have

$$\dot{p}_i = e\,(\boldsymbol{v}\times\boldsymbol{B})_i + e\,\frac{d\,A_i}{d\,t} - \partial_i V$$

$$\to \qquad \frac{d}{d\,t}(p_i - e\,A_i) = e\,(\boldsymbol{v}\times\boldsymbol{B})_i - \partial_i V$$

$$m\,\dot{\boldsymbol{v}} = e\,\boldsymbol{v}\times\boldsymbol{B} - \nabla V \tag{3.13a}$$

Under a gauge transformation

$$\boldsymbol{A} \;\to\; \boldsymbol{A}' = \boldsymbol{A} + \nabla\Lambda(\boldsymbol{q})$$

we have

$$\boldsymbol{B} \;\to\; \boldsymbol{B}' = \nabla\times\boldsymbol{A}' = \nabla\times\boldsymbol{A} = \boldsymbol{B} \qquad (\,\nabla\times\nabla\Lambda = \epsilon_{ijk}\,\partial_j\partial_k V = 0\,)$$

while the equation of motion takes the same form as eq(3.13a) but with

$$\boldsymbol{v} = \frac{1}{m}(\boldsymbol{p} - e\,\boldsymbol{A}') = \frac{1}{m}(\boldsymbol{p} - e\,\boldsymbol{A} - e\,\nabla\Lambda)$$

This form invariance of the equation of motion is usually referred to as the gauge invariance of H (or the Lagrangian L).

3.2.1. Quantization in a Magnetic Field

The quantized version of eq(3.13) is simply

$$H = \frac{1}{2\,m}\left[\hat{\boldsymbol{p}} - e\,\boldsymbol{A}(\hat{\boldsymbol{q}})\right]^2 + V(\hat{\boldsymbol{q}})$$

$$= \frac{1}{2\,m}\left[\hat{\boldsymbol{p}}^2 - e\,\boldsymbol{A}(\hat{\boldsymbol{q}})\cdot\hat{\boldsymbol{p}} - e\,\hat{\boldsymbol{p}}\cdot\boldsymbol{A}(\hat{\boldsymbol{q}}) + e^2\,\boldsymbol{A}^2\right] + V(\hat{\boldsymbol{q}}) \tag{3.14}$$

for which the issue of the ordering of the $\hat{\boldsymbol{p}}$, $\hat{\boldsymbol{q}}$ operators never arise.

Analogeous to the classical case, gauge invariance of H here means the form invariance of the Schrodinger equation

$$H\psi = E\psi$$

In the q-representation, we have

$$H = \frac{1}{2m}[-i\hbar\nabla - e\boldsymbol{A}(\boldsymbol{q})]^2 + V(\boldsymbol{q})$$

$$\rightarrow \qquad H\psi = \frac{1}{2m}(-i\hbar\nabla - e\boldsymbol{A})\cdot(-i\hbar\nabla\psi - e\boldsymbol{A}\psi)$$

$$= \frac{1}{2m}\left[-\hbar^2\nabla^2\psi + ie\hbar\boldsymbol{A}\cdot\nabla\psi + ie\hbar\nabla\cdot(\boldsymbol{A}\psi) + e^2\boldsymbol{A}^2\psi\right]$$

$$= \frac{1}{2m}\left[-\hbar^2\nabla^2\psi + 2ie\hbar\boldsymbol{A}\cdot\nabla\psi + ie\hbar(\nabla\cdot\boldsymbol{A})\psi + e^2\boldsymbol{A}^2\psi\right]$$

$$\therefore \qquad H = \frac{1}{2m}\left(-\hbar^2\nabla^2 + 2ie\hbar\boldsymbol{A}\cdot\nabla + ie\hbar\,\nabla\cdot\boldsymbol{A} + e^2\boldsymbol{A}^2\right) + V$$

where ∇ is understood to operate only on what is immediately adjacent to it, i.e.,

$$\nabla A\,B = (\nabla A)\,B$$

Under the gauge transformation

$$\boldsymbol{A} \rightarrow \boldsymbol{A}' = \boldsymbol{A} + \nabla\Lambda(\boldsymbol{q}) \tag{3.16}$$

we have

$$H \rightarrow H' = H + i\frac{e\hbar}{m}\nabla\Lambda\cdot\nabla + i\frac{e\hbar}{2m}\nabla^2\Lambda + \frac{e^2}{2m}\left[2\boldsymbol{A}\cdot\nabla\Lambda + (\nabla\Lambda)^2\right]$$

$$\psi(\boldsymbol{q}) \rightarrow \psi'(\boldsymbol{q}) = e^{i\chi(\boldsymbol{q})}\psi(\boldsymbol{q})$$

where χ is real if ψ' is to have the same local physical properties as ψ.

Using

$$\nabla\psi' = e^{i\chi}(i\psi\nabla\chi + \nabla\psi)$$

$$\nabla^2\psi' = \nabla\cdot\left[e^{i\chi}(i\psi\nabla\chi + \nabla\psi)\right]$$

$$= e^{i\chi}\left[i\nabla\chi\cdot(i\psi\nabla\chi + \nabla\psi) + i\nabla\psi\cdot\nabla\chi + i\psi\nabla^2\chi + \nabla^2\psi\right]$$

$$= e^{i\chi}\left[-\psi(\nabla\chi)^2 + 2i\nabla\chi\cdot\nabla\psi + i\psi\nabla^2\chi + \nabla^2\psi\right]$$

we have

$$H\psi' = e^{i\chi}\left\{H\psi - \frac{\hbar^2}{2m}\left[-\psi(\nabla\chi)^2 + 2i\nabla\chi\cdot\nabla\psi + i\psi\nabla^2\chi\right] - \frac{e\hbar}{m}\psi\boldsymbol{A}\cdot\nabla\chi\right\}$$

$$\rightarrow \qquad H'\psi' = H\psi' + e^{i\chi}\left\{-\frac{e\hbar}{m}\psi\nabla\Lambda\cdot\nabla\chi\right.$$

$$\left. + i\frac{e\hbar}{m}\nabla\Lambda\cdot\nabla\psi + i\frac{e\hbar}{2m}\psi\nabla^2\Lambda + \frac{e^2}{2m}\left[2\boldsymbol{A}\cdot\nabla\Lambda + (\nabla\Lambda)^2\right]\psi\right\}$$

$$= e^{i\chi}\left\{H\psi - \frac{\hbar^2}{2m}\left[-\psi(\nabla\chi)^2 + 2i\nabla\chi\cdot\nabla\psi + i\psi\nabla^2\chi\right] - \frac{e\hbar}{m}\psi(\boldsymbol{A} + \nabla\Lambda)\cdot\nabla\chi\right.$$

$$\left. + i\frac{e\hbar}{m}\nabla\Lambda\cdot\nabla\psi + i\frac{e\hbar}{2m}\psi\nabla^2\Lambda + \frac{e^2}{2m}\left[2\boldsymbol{A}\cdot\nabla\Lambda + (\nabla\Lambda)^2\right]\psi\right\}$$

Setting

$$\chi = \frac{e}{\hbar}\Lambda$$

we have

$$H'\,\psi' = e^{i\chi}\left\{ H\,\psi + \frac{e^2}{2m}\,\psi\,(\nabla\Lambda)^2 - i\,\frac{e\,\hbar}{m}\,\nabla\Lambda\cdot\nabla\psi - i\,\frac{e\,\hbar}{2m}\,\psi\,\nabla^2\Lambda - \frac{e^2}{m}\,\psi\,(\boldsymbol{A}+\nabla\Lambda)\cdot\nabla\Lambda \right.$$
$$\left. + \,i\,\frac{e\,\hbar}{m}\,\nabla\Lambda\cdot\nabla\psi + i\,\frac{e\,\hbar}{2m}\,\psi\,\nabla^2\Lambda + \frac{e^2}{m}\,\psi\,\boldsymbol{A}\cdot\nabla\Lambda + \frac{e^2}{2m}\,(\nabla\Lambda)^2\,\psi \right\}$$
$$= e^{i\chi}\,H\,\psi$$
$$= e^{i\chi}\,E\,\psi$$
$$= E\,\psi'$$

Thus, setting

$$\psi \;\to\; \psi' = \psi\,\exp\!\left(i\,\frac{e}{\hbar}\,\Lambda\right) \qquad (3.15)$$

will leave the Schrodinger equation invariant.

The Lagrangian associated with eq(3.14) is

$$L = \boldsymbol{p}\cdot\boldsymbol{v} - H = (m\,\boldsymbol{v} + e\,\boldsymbol{A})\cdot\boldsymbol{v} - \left(\frac{1}{2}\,m\,\boldsymbol{v}^2 + V\right)$$
$$= \frac{1}{2}\,m\,\boldsymbol{v}^2 + e\,\boldsymbol{A}\cdot\boldsymbol{v} - V \qquad \text{(real time)}$$
$$= -\frac{1}{2}\,m\,\dot{\boldsymbol{q}}^2 + i\,e\,\boldsymbol{A}\cdot\dot{\boldsymbol{q}} - V \qquad \text{(imaginary time)} \qquad (3.17a)$$

A direct solution to eq(3.1 or 2.7) in discretized form is [see eqs(2.16 & 2.34a)]

$$\langle \boldsymbol{q}'' \mid U(t'',\,t') \mid \boldsymbol{q}' \rangle_\varepsilon = \lim_{n\to\infty}\left(\frac{m}{2\,\pi\,\hbar\,\varepsilon}\right)^{3n/2} \int \prod_{k=1}^{n-1} d\,\boldsymbol{q}_k\,\exp\!\left(-\frac{1}{\hbar}\,S[\boldsymbol{q},\,\varepsilon]\right)$$

where

$$S[\boldsymbol{q},\,\varepsilon] = \varepsilon\,\sum_{k=1}^{n}\left[\frac{1}{2}\,m\left(\frac{q_k - q_{k-1}}{\varepsilon}\right)^2 + V(q_k)\right] \qquad \text{(imaginary time)}$$
$$\to\; -\int_{t'}^{t''} d\,t\,L$$

In the presence of a magnetic field, eq(3.17a) indicates an extra contribution to S given by

$$-i\,e\int_{t'}^{t''} d\,t\,\boldsymbol{A}\cdot\dot{\boldsymbol{q}} \qquad (3.17b)$$

To discretize eq(3.17b), we divide the integral into n intervals so that in the k^{th} interval, $\boldsymbol{q}$ changes from $\boldsymbol{q}_{k-1}$ to $\boldsymbol{q}_k$. Assuming a linear change, we set

$$\boldsymbol{q}_k(s) = (1-s)\,\boldsymbol{q}_{k-1} + s\,\boldsymbol{q}_k \qquad s\in[0,\,1]$$

so that

$$\boldsymbol{q}_k(0) = \boldsymbol{q}_{k-1} \qquad \& \qquad \boldsymbol{q}_k(1) = \boldsymbol{q}_k$$

With

$$d\,t = \varepsilon\,d\,s \qquad \& \qquad \dot{\boldsymbol{q}}_k \approx \frac{\boldsymbol{q}_k - \boldsymbol{q}_{k-1}}{\varepsilon}$$

eq(3.17b) becomes

$$-i\,e\int_{t'}^{t''} d\,t\,\boldsymbol{A}\cdot\dot{\boldsymbol{q}} = -i\,e\,\sum_{k=1}^{n}\int_0^1 d\,s\;\boldsymbol{A}[\boldsymbol{q}_k(s)]\cdot(\boldsymbol{q}_k - \boldsymbol{q}_{k-1}) \qquad (3.17)$$

A non-linear choice of $\boldsymbol{q}_k(s)$ may lead to a non-hermitian quantization of H. [See zinn-Justin]

If we use the general action eq(3.8), we get

$$S(\boldsymbol{p},\,\boldsymbol{q}) = \int_{t'}^{t''} d\,t \left\{ -i\,\boldsymbol{p}\cdot\dot{\boldsymbol{q}} + \frac{(\boldsymbol{p} - e\,\boldsymbol{A})^2}{2\,m} + V \right\} \tag{3.18a}$$

On the classical path, we have

$$\boldsymbol{p} = i\,m\,\dot{\boldsymbol{q}} + e\,\boldsymbol{A}$$

Therefore, we set

$$\boldsymbol{p} = i\,m\,\dot{\boldsymbol{q}} + e\,\boldsymbol{A} + \boldsymbol{r}$$

$$\rightarrow \qquad \frac{(\boldsymbol{p} - e\,\boldsymbol{A})^2}{2\,m} = \frac{1}{2\,m}(i\,m\,\dot{\boldsymbol{q}} + \boldsymbol{r})^2$$

$$= -\frac{1}{2}\,m\,\dot{\boldsymbol{q}}^2 + i\,\dot{\boldsymbol{q}}\cdot\boldsymbol{r} + \frac{1}{2}\,m\,\boldsymbol{r}^2$$

$$-i\,\boldsymbol{p}\cdot\dot{\boldsymbol{q}} = m\,\dot{\boldsymbol{q}}^2 - i\,e\,\boldsymbol{A}\cdot\dot{\boldsymbol{q}} - i\,\boldsymbol{r}\cdot\dot{\boldsymbol{q}}$$

$$\therefore \qquad S(\boldsymbol{r},\,\boldsymbol{q}) = \int_{t'}^{t''} d\,t \left\{ \frac{1}{2}\,m\,\dot{\boldsymbol{q}}^2 - i\,e\,\boldsymbol{A}\cdot\dot{\boldsymbol{q}} + \frac{1}{2}\,m\,\boldsymbol{r}^2 + V \right\} \tag{3.18b}$$

Thus, the integral over momentum $\boldsymbol{r}$ remains a Gaussian like the non-magnetic case. After it's done, we get

$$S(\boldsymbol{q}) = \int_{t'}^{t''} d\,t \left(\frac{1}{2}\,m\,\dot{\boldsymbol{q}}^2 - i\,e\,\boldsymbol{A}\cdot\dot{\boldsymbol{q}} + V \right) \tag{3.18}$$

which is simply the continuum limit of the discretized result.

Under a guage transformation

$$\boldsymbol{A} \;\rightarrow\; \boldsymbol{A}' = \boldsymbol{A} + \nabla\Lambda$$

the change in S is

$$\delta\,S = -i\,e\int_{t'}^{t''} d\,t\,\nabla\,\Lambda\cdot\dot{\boldsymbol{q}}$$

$$= -i\,e\int_{\boldsymbol{q}(t')}^{\boldsymbol{q}(t'')} d\,\boldsymbol{q}\cdot\nabla\,\Lambda$$

$$= -i\,e\int_{\Lambda[\boldsymbol{q}(t')]}^{\Lambda[\boldsymbol{q}(t'')]} d\,\Lambda$$

$$= -i\,e\,[\Lambda(\boldsymbol{q}'') - \Lambda(\boldsymbol{q}')]$$

Hence, $\langle\,\boldsymbol{q}''\mid U(t'',\,t')\mid \boldsymbol{q}'\,\rangle$ gains a factor $\exp\left\{\frac{i}{\hbar}\,e[\Lambda(\boldsymbol{q}'') - \Lambda(\boldsymbol{q}')]\right\}$, in agreement with the transformation law eq(3.15).

Hermiticity & the $\varepsilon(0)$ Problem

Consider a harmonic oscillator coupled to a magnetic field. Eq(3.18) becomes

$$S(\boldsymbol{q}) = \int d\,t \left(\frac{1}{2}\,m\,\dot{\boldsymbol{q}}^2 - i\,e\,\boldsymbol{A}\cdot\dot{\boldsymbol{q}} + \frac{1}{2}\,m\,\omega^2\,\boldsymbol{q}^2 \right)$$

together with the path integral

$$\mathcal{I} = \int [d\,\boldsymbol{q}]\,e^{-S/\hbar}$$

Let

$$S = S_0 - i\,e\int d\,t\,\boldsymbol{A}\cdot\dot{\boldsymbol{q}} \quad \text{with} \qquad S_0 = \int d\,t \left(\frac{1}{2}\,m\,\dot{\boldsymbol{q}}^2 + \frac{1}{2}\,m\,\omega^2\,\boldsymbol{q}^2 \right)$$

$$\rightarrow \qquad \mathcal{I} = \int [d\,\boldsymbol{q}]\,e^{-S_0/\hbar}\left(1 + i\,\frac{e}{\hbar}\int d\,t\,\boldsymbol{A}\cdot\dot{\boldsymbol{q}} + \dots \right)$$

$$= \mathcal{I}_0 + i\,\frac{e}{\hbar}\left\langle \int d\,t\,\boldsymbol{A}\cdot\dot{\boldsymbol{q}} \right\rangle + \ldots$$

where

$$\mathcal{I}_0 = \int [d\,\boldsymbol{q}]\, e^{-S_0/\hbar}$$

$$\langle X \rangle \equiv \frac{1}{\mathcal{I}_0} \int [d\,\boldsymbol{q}]\, e^{-S_0/\hbar}\, X$$

$$\int d\,t\,\boldsymbol{A}\cdot\dot{\boldsymbol{q}} = \int d\,\boldsymbol{q}\cdot\boldsymbol{A}$$

$$= -\int \boldsymbol{q}\cdot d\,\boldsymbol{A} \qquad (\ \boldsymbol{q} \text{ and/or } \boldsymbol{A} = 0 \text{ at boundaries assumed })$$

$$= -\int q_i\, \frac{\partial A_i}{\partial q_j}\, \frac{d\,q_j}{d\,t}\, d\,t$$

$$\to \qquad \mathcal{I} = \mathcal{I}_0 - i\,\frac{e}{\hbar}\int d\,t \left\langle q_i\, \frac{\partial A_i}{\partial q_j}\, \dot{q}_j \right\rangle + \ldots$$

$$= \mathcal{I}_0 - i\,\frac{e}{\hbar}\int d\,t \left\langle q_i(t)\, \dot{q}_j(t) \right\rangle \left\langle \frac{\partial A_i}{\partial q_j} \right\rangle + \ldots \qquad \text{(Wick's theorem used)}$$

Generalizing the 1-D harmonic oscillator results in §2.5, namely,

$$\langle\, q(t_1)\, q(t_2)\,\rangle = \frac{\hbar}{m}\,\Delta(t_1 - t_2) \qquad (2.48b)$$

$$\Delta(t) = \frac{1}{2\,\omega}\, e^{-\omega\,|t|} \qquad (2.46)$$

we set

$$\left\langle q_i\,(t_1)\, q_j\,(t_2) \right\rangle = \delta_{i\,j}\, \frac{\hbar}{m}\,\Delta(t_1 - t_2)$$

$$\to \qquad \left\langle q_i\,(t_1)\, \dot{q}_j\,(t_2) \right\rangle = \delta_{i\,j}\, \frac{\hbar}{m}\, \frac{d}{d\,t_2}\,\Delta(t_1 - t_2)$$

$$= \delta_{i\,j}\, \frac{\hbar}{2\,m\,\omega}\, \frac{d}{d\,t_2}\, e^{-\omega\,|t_1 - t_2|}$$

$$= \delta_{i\,j}\, \frac{\hbar}{2\,m} \begin{cases} e^{-\omega\,(t_1 - t_2)} & \text{for } \ t_1 > t_2 \\ -e^{-\omega\,(t_2 - t_1)} & \text{for } \ t_2 > t_1 \end{cases}$$

$$= \delta_{i\,j}\, \frac{\hbar}{2\,m}\, e^{-\omega\,|t_1 - t_2|}\, \epsilon(t_1 - t_2) \qquad (3.18c)$$

where

$$\epsilon(t) = \begin{cases} 1 & \text{for } \ t > 0 \\ -1 & \text{for } \ t < 0 \end{cases}$$

is the sign function.

Hence, formally,

$$\mathcal{I} = \mathcal{I}_0 - i\,\frac{e}{2\,m}\,\epsilon(0) \int d\,t \left\langle \frac{\partial A_j}{\partial q_j} \right\rangle + \ldots$$

$$= \mathcal{I}_0 - i\,\frac{e}{2\,m}\,\epsilon(0) \int d\,t\, \langle \nabla\cdot\boldsymbol{A} \rangle + \ldots$$

except that $\epsilon(0)$ is not uniquely defined.

If $\mathcal{I}$ is to be time-reversal invariant, the term odd in t must vanish, which means we must set $\epsilon(0) = 0$.

Furthermore,

$$\frac{d}{dt}\left\langle q_i(t)\, q_j(t)\right\rangle = \lim_{t_1 \to t_2}\left\{\left\langle \dot{q}_i(t_1)\, q_j(t_2)\right\rangle + \left\langle q_i(t_1)\, \dot{q}_j(t_2)\right\rangle\right\}$$

$$= \lim_{t_1 \to t_2} \delta_{ij}\frac{\hbar}{2m}\begin{cases} -e^{-\omega(t_1-t_2)} + e^{-\omega(t_1-t_2)} & \text{for } t_1 > t_2 \\ e^{-\omega(t_2-t_1)} - e^{-\omega(t_2-t_1)} & \text{for } t_2 > t_1 \end{cases}$$

$$= 0$$

while eq(3.18c) gives

$$\lim_{t_1 \to t_2}\left\langle q_i(t_1)\, \dot{q}_j(t_2)\right\rangle = \lim_{t_1 \to t_2}\left\langle \dot{q}_i(t_1)\, q_j(t_2)\right\rangle = \delta_{ij}\frac{\hbar}{2m}\epsilon(0)$$

so that

$$\frac{d}{dt}\left\langle q_i(t)\, q_j(t)\right\rangle = \delta_{ij}\frac{\hbar}{m}\epsilon(0)$$

Therefore, only the choice $\varepsilon(0) = 0$ is consistent with the commutation between time derivative and averaging.

See Zinn-Justin's text for discussions on how the choice $\varepsilon(0) = 0$ also preserves the hermiticity of $e^{-\beta H}$. Hint: time reversal becomes exchange of B.C.'s at $t = 0$ & $\hbar\beta$ & hence transposition of S taken as a matrix.

3.2.2. General Quadratic Hamiltonian

Consider the problem of quantizing a general real time Lagrangian quadratic in $\dot{q}$.

$$L(q, \dot{q}) = \frac{1}{2} g_{\alpha\beta}(q)\, \dot{q}^\alpha \dot{q}^\beta - h_\alpha(q)\, \dot{q}^\alpha - v(q) \tag{3.19}$$

where $g_{\alpha\beta}(q)$ is a symmetric & positive matrix. For motions on a Riemannian manifold, $g_{\alpha\beta}$ is the metric tensor (hence the upper & lower indices for contravariant & covariant components, respectively).

The conjugate momenta are

$$p_\alpha = \frac{\partial L}{\partial \dot{q}^\alpha} = \frac{1}{2}\left(g_{\mu\nu}\,\delta^\mu_\alpha\, \dot{q}^\nu + g_{\mu\nu}\, \dot{q}^\mu\, \delta^\nu_\alpha\right) - h_\mu\, \delta^\mu_\alpha$$

$$= \frac{1}{2}\left(g_{\alpha\nu}\, \dot{q}^\nu + g_{\mu\alpha}\, \dot{q}^\mu\right) - h_\alpha$$

$$= g_{\alpha\beta}\, \dot{q}^\beta - h_\alpha$$

$$\rightarrow \qquad g^{\alpha\mu}\, p_\mu = g^{\alpha\mu}\, g_{\mu\beta}\, \dot{q}^\beta - g^{\alpha\mu}\, h_\mu$$

By definition,

$$g^{\alpha\mu}\, g_{\mu\beta} = \delta^\alpha_\beta$$

therefore

$$\dot{q}^\alpha = g^{\alpha\mu}(p_\mu + h_\mu)$$

The hamiltonian is given by the Legendre transform

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

$$= \frac{1}{2} g_{\alpha\beta}\, \dot{q}^\alpha \dot{q}^\beta + v$$

$$= \frac{1}{2} g_{\alpha\beta}\, g^{\alpha\mu}(p_\mu + h_\mu)\, g^{\beta\nu}(p_\nu + h_\nu) + v$$

$$= \frac{1}{2}\left(p_\beta + h_\beta\right) g^{\beta\nu} (p_\nu + h_\nu) + v$$
$$= \frac{1}{2}\left(p_\alpha + h_\alpha\right) g^{\alpha\beta} \left(p_\beta + h_\beta\right) + v \tag{3.20}$$

Generalizing eq(3.5) to the 3-D case, we have

$$\langle \boldsymbol{q} \mid U(t, t-\varepsilon) \mid \boldsymbol{q}' \rangle = \int \frac{d^3 p}{(2\pi\hbar)^3} \exp\left\{ \frac{\varepsilon}{\hbar}\left[\frac{i}{\varepsilon} p_\alpha (q-q')^\alpha - \frac{1}{2}\left[p_\alpha + h_\alpha(q_{\text{av}}) \right] g^{\alpha\beta}(q_{\text{av}}) \left[p_\beta + h_\beta(q_{\text{av}}) \right] - v(q_{\text{av}}) \right] \right\} \tag{3.21}$$

Note that zinn-Justin uses $\frac{d p}{2\pi\hbar}$ instead of $\frac{d^3 p}{(2\pi\hbar)^3}$.

Let

$$P_\alpha = p_\alpha + h_\alpha \qquad\qquad d P_\alpha = d p_\alpha$$

$$\rightarrow \qquad \langle q \mid U(t, t-\varepsilon) \mid q' \rangle = \exp\left\{ -\frac{\varepsilon}{\hbar}\left[\frac{i}{\varepsilon} h_\alpha(q_{\text{av}}) (q-q')^\alpha + v(q_{\text{av}}) \right] \right\} \mathcal{G}$$

where

$$\mathcal{G} = \int \frac{d^3 p}{(2\pi\hbar)^3} \exp\left\{ \frac{\varepsilon}{\hbar}\left[-\frac{1}{2} P_\alpha g^{\alpha\beta}(q_{\text{av}}) P_\beta + \frac{i}{\varepsilon} P_\alpha (q-q')^\alpha \right] \right\}$$

$\mathcal{G}$ can be evaluated by the formula eq(1.8)

$$\int d^n x \exp\left(-\frac{1}{2} \boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x} + \boldsymbol{b}^T \boldsymbol{x} \right) = \frac{(2\pi)^{n/2}}{\sqrt{\det \boldsymbol{A}}} \exp\left(\frac{1}{2} \boldsymbol{b}^T \boldsymbol{A}^{-1} \boldsymbol{b} \right)$$

by setting

$$\boldsymbol{x} = \sqrt{\frac{\varepsilon}{\hbar}}\, \boldsymbol{P} \qquad \boldsymbol{A} = g^{\alpha\beta} = \left(g_{\alpha\beta}\right)^{-1} \equiv \boldsymbol{g}^{-1} \qquad \boldsymbol{b} = \frac{i}{\sqrt{\hbar\varepsilon}} (\boldsymbol{q} - \boldsymbol{q}')$$

we get

$$\mathcal{G} = \left(\frac{1}{2\pi\hbar\varepsilon} \right)^{3/2} \sqrt{\det \boldsymbol{g}}\, \exp\left[-\frac{1}{2\hbar\varepsilon} (\boldsymbol{q}-\boldsymbol{q}')^T \boldsymbol{g} (\boldsymbol{q}-\boldsymbol{q}') \right]$$

so that

$$\langle \boldsymbol{q} \mid U(t, t-\varepsilon) \mid \boldsymbol{q}' \rangle = \left(\frac{1}{2\pi\hbar\varepsilon} \right)^{3/2} \sqrt{\det \boldsymbol{g}}\, \exp\left[-\frac{1}{\hbar} S(\boldsymbol{q}, \boldsymbol{q}'; \varepsilon) \right] \tag{3.22a}$$

with

$$S(\boldsymbol{q}, \boldsymbol{q}'; \varepsilon) = \varepsilon\left[i\, h_\alpha(q_{\text{av}}) \frac{(q-q')^\alpha}{\varepsilon} + v(q_{\text{av}}) + \frac{1}{2} \frac{(q-q')^\alpha}{\varepsilon} g_{\alpha\beta}(q_{\text{av}}) \frac{(q-q')^\beta}{\varepsilon} \right] \tag{3.22}$$

In the continuum limit, we have [see eq(3.7)]

$$S(\boldsymbol{q}) = \lim_{\varepsilon\to 0} \sum_{k=1}^{n} S(\boldsymbol{q}_k, \boldsymbol{q}_{k-1}; \varepsilon)$$
$$= \int_{t'}^{t''} d t \left[i\, h_\alpha\, \dot{q}^\alpha + v(\boldsymbol{q}) + \frac{1}{2} \dot{q}^\alpha g_{\alpha\beta}(\boldsymbol{q}) \dot{q}^\beta \right] \tag{3.23}$$
$$= -\int_{t'}^{t''} d t\, L$$

where, as expected, L is the imaginary time version of eq(3.19).

Similarly, eq(3.22a) becomes

$$\langle \boldsymbol{q}'' \mid U(t'', t') \mid \boldsymbol{q}' \rangle = \int [d\,q]\, \mathcal{N}(\boldsymbol{q}) \exp\left[-\frac{1}{\hbar} S(\boldsymbol{q})\right] \tag{3.24}$$

where

$$\mathcal{N}(\boldsymbol{q}) = \lim_{\substack{n\to\infty \\ \varepsilon\to 0}} (2\pi\hbar\varepsilon)^{-3n/2} \prod_{k=1}^{n} \sqrt{\det \boldsymbol{g}(\boldsymbol{q}_k)}$$

$$= \lim_{\substack{n\to\infty \\ \varepsilon\to 0}} (2\pi\hbar\varepsilon)^{-3n/2} \exp\left[\frac{1}{2}\sum_{k=1}^{n} \ln\det \boldsymbol{g}(\boldsymbol{q}_k)\right] \tag{3.25}$$

$$= \lim_{\substack{n\to\infty \\ \varepsilon\to 0}} (2\pi\hbar\varepsilon)^{-3n/2} \exp\left(\frac{1}{2\varepsilon}\int_{t'}^{t''} d\,t \ln\det \boldsymbol{g}[\boldsymbol{q}(t)]\right) \tag{3.26}$$

$$= \lim_{\substack{n\to\infty \\ \varepsilon\to 0}} (2\pi\hbar\varepsilon)^{-3n/2} \exp\left(\frac{1}{2\varepsilon}\int_{t'}^{t''} d\,t\, \mathrm{tr} \ln \boldsymbol{g}[\boldsymbol{q}(t)]\right) \tag{3.27}$$

where we've used [see eq(1.101)]

$$\ln\det \boldsymbol{M} = \mathrm{tr}\ln \boldsymbol{M}$$

See Zinn-Justin's text for some important technical issues.