Appendix E

Covariant Classical and Quantum Mechanins

E.1 Conventional Mechanics

E.1.1 Action Principle for Several Dependent variables

A dynamic system with m degrees of freedom describes the evolution in time t of m Lagrangian variables q^i, where $i = 1, \ldots, m$. We denote the space in which the variables q^i take value is a $m-$dimensional configuration space $\mathcal{C}_0$.

The dynamics of the system is determined by the Lagrangian $\mathcal{L}$ which is a function of several dependent variables $q^1(t), \ldots, q^m(t)$ and $\dot{q}^1(t), \ldots, \dot{q}^m(t)$ all of which depend on t, the independent variable.

Given two times t_1 and t_2 and two points q_1^i and q_2^i in $\mathcal{C}_0$, physical motions are such that the action

$$S[q] = \int_{t_1}^{t_2} dt \, \mathcal{L}\left(q^i(t), \frac{dq^(t)}{dt}\right) \tag{E.1}$$

is an extremum in the space of motions $q^i(t)$ such that $q^i(t_1) = q_1^i$ and $q^i(t_2) = q_2^i$. Physical motions satisfy the Euler-Lagrange equations, which we derive now.

We compare neighbouring paths by writing

$$q^i(t;\alpha) = q^i(t;0) + \alpha\eta^i(t), \qquad i = 1, 2, \ldots, m, \tag{E.2}$$

where the η_i are independent, but subject them to the condition

$$\eta^i(t_1) = \eta^i(t_2) = 0, \qquad i = 1, 2, \ldots, m. \tag{E.3}$$

Differentiating with respect to α and setting $\alpha = 0$ we obtain

$$\int_{t_1}^{t_2} \sum_i \left[\frac{\partial \mathcal{L}}{\partial q^i} \eta^i(t) + \frac{\partial \mathcal{L}}{\partial q_t^i} \frac{d\eta^i(t)}{dt} \right] dt = 0. \tag{E.4}$$

Integrating by parts

$$\int_{t_1}^{t_2} \sum_i \left[\frac{\partial \mathcal{L}}{\partial q^i} - \frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial q_t^i} \right) \right] \eta^i(t) dt + \sum_i \left[\frac{\partial \mathcal{L}}{\partial q_t^i} \eta^i(t) \right]_{t_1}^{t_2} = 0. \tag{E.5}$$

Inserting (E.3) into this we have

$$\int_{t_1}^{t_2} \sum_i \left[\frac{\partial \mathcal{L}}{\partial q^i} - \frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial q_t^i} \right) \right] \eta^i(t) dt = 0. \tag{E.6}$$

Since the η^i are arbitrary and independent of each other, each of the terms vanishes independently

$$\frac{\partial \mathcal{L}}{\partial q^i} - \frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial q_t^i} \right) = 0, \qquad i = 1, 2, \ldots, m. \tag{E.7}$$

These are the Euler-Lagrange equations. A dynamical system is therefore specified by the couple $(\mathcal{C}_0, \mathcal{L})$.

E.1.2 The Hamilton Equations

The Hamiltonian from a Lagrangian

The momenta are calculated by differentiating the Lagrangian via

$$p_i(q^i, \dot{q}^i, t) = \frac{\partial \mathcal{L}}{\partial \dot{q}^i}. \tag{E.8}$$

Inverting the function $p_i(q^i, \dot{q}^i)$ yields the function $\dot{q}^i(q^i, p_i)$. Defing the Hamiltonian by

$$
\begin{aligned}
H_0(q^i, p_i) &= \frac{\partial \mathcal{L}}{\partial \dot{q}^i}\dot{q}(q^i, p_i) - \mathcal{L}(q^i, \dot{q}(q^i, p_i)) \\
&= p_i \dot{q}(q^i, p_i) - \mathcal{L}(q^i, \dot{q}(q^i, p_i)).
\end{aligned} \tag{E.9}
$$

We derive Hamilton's equations by considering the total derivative of the Lagrangian

$$
d\mathcal{L} = \sum_i \left(\frac{\partial \mathcal{L}}{\partial q^i} dq^i + \frac{\partial \mathcal{L}}{\partial \dot{q}^i} d\dot{q}^i \right) + \frac{\partial \mathcal{L}}{\partial t} dt. \tag{E.10}
$$

We substitute (E.8) into the total differential of the Lagrangian

$$
d\mathcal{L} = \sum_i \left(\frac{\partial \mathcal{L}}{\partial q^i} dq^i + p_i d\dot{q}^i \right) + \frac{\partial \mathcal{L}}{\partial t} dt. \tag{E.11}
$$

This can then be written as

$$
d\mathcal{L} = \sum_i \left(\frac{\partial \mathcal{L}}{\partial q^i} dq^i + d(p_i \dot{q}^i) - \dot{q}^i dp_i \right) + \frac{\partial \mathcal{L}}{\partial t} dt, \tag{E.12}
$$

which after rearangment becomes

$$
d \left(\sum_i p_i \dot{q}^i - \mathcal{L} \right) = \sum_i \left(-\frac{\partial \mathcal{L}}{\partial q^i} dq^i + \dot{q}^i dp_i \right) - \frac{\partial \mathcal{L}}{\partial t} dt. \tag{E.13}
$$

The term on the LHS is the Hamiltonian, therefore

$$
dH_0 = \sum_i \left(-\frac{\partial \mathcal{L}}{\partial q^i} dq^i + \dot{q}^i dp_i \right) - \frac{\partial \mathcal{L}}{\partial t} dt. \tag{E.14}
$$

We now consider the total derivative of the Hamiltonian

$$
dH_0 = \sum_i \left(\frac{\partial H_0}{\partial q^i} dq^i + \frac{\partial H_0}{\partial p_i} dp_i \right) + \frac{\partial H_0}{\partial t} dt. \tag{E.15}
$$

Comparing the terms of (E.14) and (E.15) give Hamilton's equations are then

$$
\begin{aligned}
\frac{dq^i(t)}{dt} &= \frac{\partial H_0(q^i,p_i)}{\partial p_i} \\
\frac{dp_i(t)}{dt} &= -\frac{\partial H_0(q^i,p_i)}{\partial q^i}
\end{aligned} \tag{E.16}
$$

and

$$
\frac{\partial H_0}{\partial t} = -\frac{\partial \mathcal{L}}{\partial t}. \tag{E.17}
$$

The $2m-$dimensional space coordinatised by the coordinates q^i and the momenta p_i is called the "conventional" phase space Γ_0.

Legendre transformations

A function $y = f(x)$ is convex if

$$
\frac{d^2 f}{dx^2} > 0 \tag{E.18}
$$

The functional relationship specified by $f(x)$ can be represented equally well as a set of tangent lines specified by their slope and intercept values. The tangent line at $x = x_0$ intersects the vertical axis at $(0, -f^*)$ and f^* is the value of the Legendre transform $f^*(p)$ where $p = \dot{f}(x_0)$.

Hamilton's equations from a variational principle

Hamilon's canonical equations can be obtained from a variational principle where we regard $q^i(t)$ and $p_i(t)$ are uncorrelated and independently adjustable functions. One abandons the formula $p_i = \partial\mathcal{L}(q^i,\dot{q}^i,t)/\partial\dot{q}^i$. Now, variations will be over paths in the (q^i,p_i) phase space, which have $2m$ dimensions.

$$
\mathcal{L}(q^i,\dot{q}^i,p_i,t) \equiv \sum_i \dot{q}^i p_i - H_0(q^i,p_i,t) \tag{E.19}
$$

(E.19) is an extremum in the space of motions in phase space (q^i,p_i) such that $q^i(t_1) = q^i_1$ and $q^i(t_2) = q^i_2$. Physical motions satisfy the Hamilton equations equations, which we derive now.

We compare neighbouring paths by writing

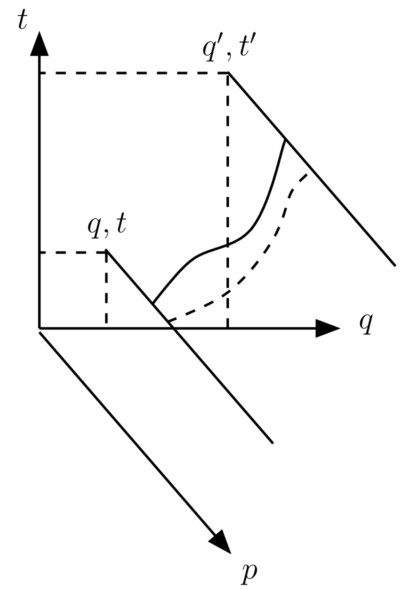

Figure E.1: We consider variations in the path that extremises (E.19) subject to the conditions that at initial time t the position is q and at final time t' the position is q'.

$$q^i(t;\alpha) = q^i(t;0) + \alpha\eta_q^i(t) \quad \text{and} \quad p_i(t;\alpha) = p_i(t;0) + \alpha\eta_{pi}(t), \quad i = 1, 2, \ldots, m, \tag{E.20}$$

where the η_q^i and η_{pi} are independent, but subject them to the condition

$$\eta_q^i(t_1) = \eta_q^i(t_2) = 0, \qquad i = 1, 2, \ldots, m. \tag{E.21}$$

Differentiating with respect to α and setting $\alpha = 0$ we obtain

$$\int_{t_1}^{t_2} \sum_i \left[\frac{\partial \mathcal{L}}{\partial q^i}\eta_q^i(t) + \frac{\partial \mathcal{L}}{\partial q_t^i}\frac{d\eta_q^i(t)}{dt} + \frac{\partial \mathcal{L}}{\partial p_i}\eta_{pi}(t) \right] dt = 0. \tag{E.22}$$

Upon substituting the RHS of (E.19) we have

$$\int_{t_1}^{t_2} \sum_i \left[-\frac{\partial H_0}{\partial q^i}\,\eta_q^i(t) + p_i\frac{d\eta_q^i(t)}{dt} + \left(\dot{q}^i - \frac{\partial H_0}{\partial p_i} \right)\eta_{pi}(t) \right] dt = 0. \tag{E.23}$$

Integrating by parts gives

$$\int_{t_1}^{t_2} \sum_i \left(-\frac{\partial H_0}{\partial q^i} - \frac{dp_i}{dt} \right) \eta_q^i(t) dt + \sum_i \left[p_i \eta_q^i(t) \right]_{t_1}^{t_2} + \int_{t_1}^{t_2} \sum_i \left(\dot{q}^i - \frac{\partial H_0}{\partial p_i} \right) \eta_{pi}(t) dt = 0. \tag{E.24}$$

Substituting in (E.21) gives

$$\int_{t_1}^{t_2} \sum_i \left(-\frac{\partial H_0}{\partial q^i} - \frac{dp_i}{dt} \right) \eta_q^i(t) dt + \int_{t_1}^{t_2} \sum_i \left(\frac{dq^i}{dt} - \frac{\partial H_0}{\partial p_i} \right) \eta_{pi}(t) dt = 0. \tag{E.25}$$

Since the η_q^i and η_{pi} are arbitrary and independent of each other, each of the terms vanishes independently,

$$\frac{dp_i}{dt} = -\frac{\partial H_0}{\partial q^i} \tag{E.26}$$

and

$$\frac{dq^i}{dt} = \frac{\partial H_0}{\partial p_i}. \tag{E.27}$$

Recovery of Second order formulism from Hamilton's equations

We now employ Hamilton's equations,

$$\frac{dq^i}{dt} = \frac{\partial H_0}{\partial p_i} \qquad \text{and} \qquad \frac{dp_i}{dt} = -\frac{\partial H_0}{\partial q^i}$$

and take $\mathcal{L}(q^i, \dot{q}^i, p_i, t) = \sum_i \dot{q}^i p_i - H_0(q^i, p_i, t)$ to recover $p_i = \partial\mathcal{L}(q^i, \dot{q}^i, t)/\partial\dot{q}^i$ together with the Euler-Lagrange equations for $\mathcal{L} = \mathcal{L}(q^i, \dot{q}^i, t)$. We write:

$$\begin{aligned} d\mathcal{L} &= \sum_i \frac{\partial\mathcal{L}}{\partial q^i} dq^i + \sum_i \frac{\partial\mathcal{L}}{\partial\dot{q}^i} d\dot{q}^i + \sum_i \frac{\partial\mathcal{L}}{\partial p_i} dp^i + \frac{\partial\mathcal{L}}{\partial t} \\ &= \sum_i p_i d\dot{q}^i + \sum_i \dot{q}^i dp_i - \sum_i \frac{\partial H_0}{\partial q^i} dq^i - \sum_i \frac{\partial H_0}{\partial p^i} dp^i - \frac{\partial H_0}{\partial t}. \end{aligned} \tag{E.28}$$

Comparing terms, and employing Hamilton's equations, we obtain:

$$
\begin{aligned}
\frac{\partial \mathcal{L}}{\partial p_i} &= \dot{q}^i - \frac{\partial H_0}{\partial p_i} = 0 \\
\frac{\partial \mathcal{L}}{\partial \dot{q}^i} &= p_i \\
\frac{\partial \mathcal{L}}{\partial q^i} &= -\frac{\partial H_0}{\partial q^i} = -\dot{p}_i
\end{aligned} \tag{E.29}
$$

The first equation implies $\mathcal{L} = \mathcal{L}(q^i, \dot{q}^i, t)$. From the second equation we recover the formula $p_i = \partial\mathcal{L}(q^i, \dot{q}^i, t)/\partial\dot{q}^i$. From the second and third equations we obtain:

$$
\frac{\partial \mathcal{L}}{\partial q^i}(q^i, \dot{q}^i, t) = \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{q}^i}(q^i, \dot{q}^i, t)\right)
$$

which is the Euler-Larange equation for $\mathcal{L}(q^i, \dot{q}^i, t)$.

E.1.3 Sympletic Geometry

Unified coordinates on $T^*\mathcal{C}_0$

Let

$$
\begin{aligned}
\xi^\mu &= (q^1, q^2 \ldots q^m, p_1, p_2 \ldots p_m) \quad \text{for} \quad (\mu = 1, \ldots, 2m) \quad \text{and} \\
\partial_\mu &= (\partial_{q^1}, \partial_{q^2}, \ldots, \partial_{q^m}, \partial_{p_1}, \partial_{p_2}, \ldots, \partial_{p_m}).
\end{aligned} \tag{E.30}
$$

Then

$$
\frac{d\xi^\mu}{dt} = \sum_{\nu=1}^{2m} \Omega^{\mu\nu} \partial_\nu \mathcal{H} \tag{E.31}
$$

$$
\{A, B\} = \sum_{\nu=1}^{2m} \partial^\mu A \Omega_{\mu\nu} \partial^\nu B := \partial_\mu A \partial^\mu B \tag{E.32}
$$

It's sort of like a scalar product. In Minkoskian spacetime the scalar product is

$$\begin{aligned} a^\mu b_\mu &= a^\mu \eta_{\mu\nu} b^\nu \\ &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \end{aligned} \tag{E.33}$$

In Hamilton mecahanics the matrix

$$\begin{pmatrix} 0_m & \mathbb{1}_m \\ -\mathbb{1}_m & 0_m \end{pmatrix} \tag{E.34}$$

plays the role η. Lorentzian tranformations leave scalar product $a^\mu b_\mu$ invariant. The transformations that leave (E.32) invariant will be the subject of the next section and are called *canonical transformations*.

Just as space and time can be treated on an equal footing in special relativity by using Minkowskian spacetime notation, the q and p variables can be treated on an equal footing by using the ξ notation introduced above.

Example 4-dimensiona phase space:

Let us check (E.30), (E.31) and (E.34) for $m = 2$:

$$\frac{d\xi^\mu}{dt} = \sum_{\nu=1}^{4} \Omega^{\mu\nu} \partial_\nu \mathcal{H}$$

reads

$$\begin{pmatrix} \frac{d\xi^1}{dt} \\ \frac{d\xi^2}{dt} \\ \frac{d\xi^3}{dt} \\ \frac{d\xi^4}{dt} \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} \begin{pmatrix} \partial_1 \mathcal{H} \\ \partial_2 \mathcal{H} \\ \partial_3 \mathcal{H} \\ \partial_4 \mathcal{H} \end{pmatrix}, \tag{E.35}$$

this gives the Hamilton equations:

$$
\begin{aligned}
\frac{d\xi^1}{dt} &= \partial_3 \mathcal{H} \quad \Longrightarrow \quad \frac{dq^1}{dt} = \frac{\partial H_0}{\partial p_1} \\
\frac{d\xi^2}{dt} &= \partial_4 \mathcal{H} \quad \Longrightarrow \quad \frac{dq^2}{dt} = \frac{\partial H_0}{\partial p_2} \\
\frac{d\xi^3}{dt} &= -\partial_1 \mathcal{H} \quad \Longrightarrow \quad \frac{dp_1}{dt} = -\frac{\partial H_0}{\partial q^1} \\
\frac{d\xi^4}{dt} &= -\partial_2 \mathcal{H} \quad \Longrightarrow \quad \frac{dp_2}{dt} = -\frac{\partial H_0}{\partial q^2}
\end{aligned}
\tag{E.36}
$$

Let us check (E.32). We have

$$
\{A, B\} = \sum_{\mu,\nu=1}^{4} \partial^\mu A \Omega_{\mu\nu} \partial^\nu B \tag{E.37}
$$

which reads

$$
\begin{aligned}
\sum_{\mu,\nu=1}^{4} \partial^\mu A \Omega_{\mu\nu} \partial^\nu B &= (\partial_1 A, \partial_2 A, \partial_3 A, \partial_4 A) \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} \begin{pmatrix} \partial_1 B \\ \partial_2 B \\ \partial_3 B \\ \partial_4 B \end{pmatrix} \\
&= \left(\partial_{q^1} A, \partial_{q^2} A, \partial_{p_1} A, \partial_{p_2} A\right) \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} \begin{pmatrix} \partial_{q^1} B \\ \partial_{q^2} B \\ \partial_{p_1} B \\ \partial_{p_2} B \end{pmatrix} \\
&= \left(\partial_{q^1} A, \partial_{q^2} A, \partial_{p_1} A, \partial_{p_2} A\right) \begin{pmatrix} \partial_{p_1 1} B \\ \partial_{p_2} B \\ -\partial_{q^1} B \\ -\partial_{q^2} B \end{pmatrix} \\
&= \left(\frac{\partial A}{\partial q^1} \frac{\partial B}{\partial p_1} - \frac{\partial A}{\partial p_1} \frac{\partial B}{\partial q^1} \right) + \left(\frac{\partial A}{\partial q^2} \frac{\partial B}{\partial p_2} - \frac{\partial A}{\partial p_2} \frac{\partial B}{\partial q^2} \right) \\
&= \{A, B\}.
\end{aligned}
\tag{E.38}
$$

□

Now, let us define for an aribrary function on phase space, f,

$$
X_0 f = v_i(q^i, p_i) \frac{\partial f}{\partial q^i} + f_i(q^i, p_i) \frac{\partial f}{\partial p_i} \tag{E.39}
$$

where

$$v_i(q^i, p_i) = \frac{\partial H_0(q^i, p_i)}{\partial p_i} \qquad f_i(q^i, p_i) = -\frac{\partial H_0(q^i, p_i)}{\partial q^i}. \tag{E.40}$$

Note

$$\begin{aligned} X_0 q^j &= v_i(q^i, p_i)\frac{\partial q^j}{\partial q^i} + f_i(q^i, p_i)\frac{\partial q^j}{\partial p_i} \\ &= \frac{\partial H_0(q^i, p_i)}{\partial p_i}\delta_{ij} \\ &= \frac{\partial H_0(q^i, p_i)}{\partial p_j} \\ &= \frac{dq^j}{dt} \end{aligned} \tag{E.41}$$

and similarly

$$\begin{aligned} X_0 p_j &= v_i(q^i, p_i)\frac{\partial p_j}{\partial q^i} + f_i(q^i, p_i)\frac{\partial p_j}{\partial p_i} \\ &= -\frac{\partial H_0(q^i, p_i)}{\partial q^j} \\ &= \frac{dp_j}{dt}. \end{aligned} \tag{E.42}$$

Time evolution is a flow $(q^i(t), p_i(t))$ in this space; we see that the vector field on Γ_0 tangent to this flow is X_0. If $f = f(q^j, p_j)$ then

$$\begin{aligned} X_0 f &= v_i(q^i, p_i)\frac{\partial f(q^j, p_j)}{\partial q^i} + f_i(q^i, p_i)\frac{\partial f(q^j, p_j)}{\partial p_i} \\ &= \frac{dq^j}{dt}\frac{\partial f(q^j, p_j)}{\partial q^j} + \frac{dp_j}{dt}\frac{\partial f(q^j, p_j)}{\partial p_j} \\ &= \frac{df(q^j, p_j)}{dt}. \end{aligned} \tag{E.43}$$

E.1.4 Canonical Transformations

We can perform a change of variables on phase space

$$\begin{aligned} Q^i &= Q^i(q^i, p_i, t) \\ P^i &= P^i(q^i, p_i, t) \end{aligned} \tag{E.44}$$

such that

$$\dot{Q}^i = \frac{\partial \mathcal{K}}{\partial P_i}, \qquad \dot{P}_i = -\frac{\partial \mathcal{K}}{\partial Q^i} \tag{E.45}$$

where $\mathcal{K}$ is the new Hamiltonian, that is it obeys Hamilton's principle

$$\delta \int_{t_1}^{t_2} \left(\sum_i P_i Q^i - \mathcal{K}(Q^i, P_i, t) \right) dt = 0. \tag{E.46}$$

It is easily seen that two Lagrangians $\mathcal{L}$ and $\mathcal{L}'$ that differ by a toal time derivative yield exactly the same equations of motion,

$$S'(q, \dot{q}) = \int_{t_1}^{t_2} dt \, \mathcal{L} = \int_{t_1}^{t_2} dt \left(\mathcal{L} + \frac{dF}{dt} \right) \tag{E.47}$$

$$\sum_i p_i \dot{q}_i - \mathcal{H} = \sum_i P_i \dot{Q}_i - \mathcal{K} + \frac{dF}{dt} \tag{E.48}$$

Which variables does F depend on?

$4m$ variables $\{q, p, Q, P\}$ $2m$ indices

$$\text{Type 1. } F_1(q^i, Q^i, t) \; (q^i, Q^i) \text{ are independent.} \tag{E.49}$$
$$\text{Type 2. } F_2(q^i, P_i, t) \; (q^i, P_i) \text{ are independent.} \tag{E.50}$$
$$\text{Type 3. } F_3(p_i, Q^i, t) \; (p_i, Q^i) \text{ are independent.} \tag{E.51}$$
$$\text{Type 4. } F_4(p_i, P_i, t) \; (p, P) \text{ are independent.} \tag{E.52}$$

Canonical transformations: Type 1

Suppose we considre a generating function of type 1:

$$F = F_1(q^i, Q^i, t). \tag{E.53}$$

Equation (E.48) is then

$$\sum_i p_i \dot{q}_i - \mathcal{H} = \sum_i P_i \dot{Q}_i - \mathcal{K} + \frac{dF_1}{dt}(q, Q). \tag{E.54}$$

We have

$$\frac{dF_1}{dt}(q, Q) = \sum_i \frac{\partial F_1}{\partial q_i}\dot{q}_i + \sum_i \frac{\partial F_1}{\partial Q_i}\dot{Q}_i + \frac{\partial F_1}{\partial t} \tag{E.55}$$

Substituting this into (E.54) gives

$$\sum_i p_i \dot{q}_i - \mathcal{H} = \sum_i P_i \dot{Q}_i - \mathcal{K} + \sum_i \frac{\partial F_1}{\partial q_i}\dot{q}_i + \sum_i \frac{\partial F_1}{\partial Q_i}\dot{Q}_i + \frac{\partial F_1}{\partial t} \tag{E.56}$$

So only two terms depend on $\dot{q}_i$ (or $\mathcal{H}$, $\mathcal{K}$) and F_1 do not depend on $\dot{q}_i$. So we may compare coefficients and obtain

$$p_i = \frac{\partial F_1}{\partial q^i} \qquad \text{for } i = 1, \ldots, m. \tag{E.57}$$

Now compare coefficients of Q_i to obtain

$$P_i = -\frac{\partial F_1}{\partial Q^i} \qquad \text{for } i = 1, \ldots, m. \tag{E.58}$$

We are then left with

$$\mathcal{K} = \mathcal{H} + \frac{\partial F_1}{\partial t}. \tag{E.59}$$

Equation (E.57) represents m relations defining the p_i as a function of q^i, Q^i, and t. Assuming that they can be inverted, we can then solve for the m Q^i's in terms of q^i, p_i, and t, thus yielding the first equation of the transformation equations (E.44). We the substitue $Q^i(q^i, p_i, t)$ into (E.58) so that they give the m P_i's as functions of q^i, p_i, and t, thus yielding the secong equation of the transformation equations (E.44).

Canonical transformations: Type 2

Suppose we considre a generating function of type 2.

$$\frac{dF_2}{dt}(q,P) = \sum_i \frac{\partial F_2}{\partial q_i}\dot{q}_i + \sum_i \frac{\partial F_2}{\partial P^i}\dot{P}^i + \frac{\partial F_2}{\partial t} \tag{E.60}$$

Inserting this into the RHS of (E.48) would not produce terms that are not likewise. So we cannot simply compare. Instead we use a Legendre transform to change variables

$$F_2(q,P,t) = F_1(q,Q,t) + \sum_i P^i Q_i \tag{E.61}$$

So replacing F_1 by $F_2 - \sum PQ$, which represents a Legendre transformation, we see:

$$\frac{dF_1}{dt} = \sum_i \frac{\partial F_2}{\partial q_i}\dot{q}_i + \frac{\partial F_2}{\partial P^i}\dot{P}^i + \frac{\partial F_2}{\partial t} - \sum_i \dot{P}^i Q_i - \sum_i P^i \dot{Q}_i \tag{E.62}$$

and so obtain

$$\sum_i p_i\dot{q}_i - \mathcal{H} = \sum_i P_i\dot{Q}_i - \mathcal{K} + \sum_i \frac{\partial F_2}{\partial q_i}\dot{q}_i + \frac{\partial F_2}{\partial P^i}\dot{P}^i + \frac{\partial F_2}{\partial t} - \sum_i \dot{P}^i Q_i - \sum_i P^i \dot{Q}_i. \tag{E.63}$$

This leads to the equations

$$p_i = \frac{\partial F_2}{\partial q^i} \qquad \text{for } i = 1, \ldots, m, \tag{E.64}$$

$$Q^i = \frac{\partial F_2}{\partial P_i} \qquad \text{for } i = 1, \ldots, m, \tag{E.65}$$

and

$$\mathcal{K} = \mathcal{H} + \frac{\partial F_2}{\partial t}. \tag{E.66}$$

Canonical transformations: Type 3 and 4

The type 3 generating function F_3 depends only on the old generalised momenta and the new generalised coordinates, in this case we use

$$F = \sum_i q^i p_i + F_3(p_i, Q^i, t). \tag{E.67}$$

We then have the equations

$$\begin{aligned} q^i &= -\frac{\partial F_3}{\partial p_i} \\ P_i &= -\frac{\partial F_3}{\partial Q^i} \\ \mathcal{K} &= H + \frac{\partial F_3}{\partial t}. \end{aligned} \tag{E.68}$$

The type 4 generating function F_3 depends only on the old and new momenta, in this case we use

$$F = \sum_i q^i p_i - \sum_i Q^i P_i + F_4(p_i, P_i, t). \tag{E.69}$$

We then have the equations

$$\begin{aligned} q^i &= -\frac{\partial F_4}{\partial p_i} \\ Q^i &= -\frac{\partial F_4}{\partial P_i} \\ \mathcal{K} &= H + \frac{\partial F_4}{\partial t}. \end{aligned} \tag{E.70}$$

E.1.5 The Hamilton-Jacobi Equation

Canonical transformations can be a way of picking phase space coordinates to simplify a problem:

$$\begin{aligned} Q &= Q(q, p, t) \\ P &= P(q, p, t) \end{aligned} \tag{E.71}$$

where Q, P are new variables and q, p are the old ones, or inversely

$$\begin{aligned} q &= q(Q, P, t) \\ p &= p(Q, P, t) \end{aligned} \tag{E.72}$$

Now, the solution to our problem is to express q and p in terms of the intial conditions q_0 and p_0 $(= q(t = 0), p(t = 0))$ and time t.

$$\begin{aligned} q &= q(q_0, p_0, t) \\ p &= p(q_0, p_0, t). \end{aligned} \tag{E.73}$$

The obvious suggestion from a comparison of (E.72) and (E.73) is to make $Q = q_0$ and $P = p_0$, i.e. the new variables equal the intial conditions. So the "motion" in the new coordinates is the system remaining staionary at a point (q_0, p_0).

Thus Hamilton's equations in the new variables are:

$$\frac{\partial \mathcal{K}}{\partial P} = \dot{Q} = \dot{q_0} = 0 \tag{E.74}$$

$$-\frac{\partial \mathcal{K}}{\partial Q} = \dot{P} = \dot{p_0} = 0 \tag{E.75}$$

This implies that $\mathcal{K}$ is equal to an arbitary functon of t - we will *choose* the simplest case:

$$\mathcal{K} = 0 \tag{E.76}$$

If $\mathcal{K} = 0$, then the original Hamiltonian must obey :

$$\mathcal{K} = 0 = H_0(q, p, t) + \frac{\partial F}{\partial t} \tag{E.77}$$

where F is the generating function of the transformation. We choose a canonical transformation as Type 1:

$$F_1(q, Q, t) \tag{E.78}$$

(though it is often choosen to be of type 2). Recall for Type 1 we have

$$\begin{aligned} \frac{\partial F_1}{\partial q} &= p, && \text{(E.79)} \\ \frac{\partial F_1}{\partial Q} &= -P && \text{(E.80)} \end{aligned}$$

and conventually (and for reasons we will see in the next section) we denote F_1 by S. To write the Hamiltonian in (E.77) in terms of the same variables, one may use (E.79). Then (E.77) becomes, with substitution of (E.79), what is called the Hamilton-Jacobi equation

$$\frac{\partial S}{\partial t} + H_0\left(q, \frac{\partial S}{\partial q}\right) = 0. \tag{E.81}$$

The Hamilton-Jacobi equation can be obtained from the classical limit of the Schrodinger equation.

E.1.6 The Hamilton Function

Let us first give the simplest example of the Hamilton function, the one with the least number of variables. The Hamilton function $S(q, t, q', t')$ is a function of four variables, q, t, q', t', defined as the action of a physical motion that starts at q at time t and ends at q' at time t'.

Let us denote $q_{qt,q't'}(\tilde{t})$ as a physical motion that starts at (q, t) and ends at (q', t'). That is, a function of time that solves the equantions of motion and such

$$\begin{aligned} q_{qt,q't'}(t) &= q, \\ q_{qt,q't'}(t') &= q'. \end{aligned} \tag{E.82}$$

Example : **Free particle**

The action is

$$S[q] = \int_t^{t'} d\tilde{t}\, \frac{1}{2} m \dot{q}^2(\tilde{t}). \tag{E.83}$$

Physical motions are straight motions

$$v \equiv \dot{q} = \frac{q' - q}{t' - t}, \tag{E.84}$$

$$
\begin{aligned}
S(q,t,q',t') &= \int_t^{t'} d\tilde{t}\, \frac{1}{2} m \left(\frac{q'-q}{t'-t} \right)^2 \\
&= \frac{m(q'-q)^2}{2(t'-t)}
\end{aligned}
\tag{E.85}
$$

where we have used that the integrand is not a function of $\tilde{t}$.

$\square$

As a worked exercise, at the end of the appendix we calculate that the Hamilton function of a harmonic oscillator is

$$
S(q,t,q',t') = m\omega \frac{(q^2 + q'^2) cos\omega(t'-t) - 2qq'}{2\sin\omega(t'-t)}
\tag{E.86}
$$

for motion that starts at (q,t) and ends at (q',t').

Definition : The Hamilton Function

Consider two points (t_1, q_1^i) and (t_2, q_2^i) in $\mathcal{C}$. The function on $\mathcal{G} = \mathcal{C} \times \mathcal{C}$

$$
S(t_1, q_1^i, t_2, q_2^i) = \int_{t_1}^{t_2} dt\, \mathcal{L}\left(q^i(t), \dot{q}^i(t)\right),
\tag{E.87}
$$

where $q^i(t)$ is the physical motion from $q_1^i(t_1)$ to $q_2^i(t_2)$.

$\square$

Properties of the Hamilton Function

Recall that the momentum is

$$
p(q,\dot{q}) = \frac{\partial \mathcal{L}(q,\dot{q})}{\partial \dot{q}}
\tag{E.88}
$$

We will prove:

$$
\frac{\partial S(q,t,q',t')}{\partial q} = -p(q,t,q',t'), \qquad \frac{\partial S(q,t,q',t')}{\partial q'} = p'(q,t,q',t')
\tag{E.89}
$$

where $p(q,t,q',t') = p(q,\dot{q}(q,t,q',t'))$ and $p'(q,t,q',t') = p'(q',\dot{q}'(q,t,q',t'))$ are the initial and final momenta respectively, expressed as functions of initial and final positions and times, via physical motions, determined by the initial and final data.

We also have

$$\frac{\partial S(q,t,q',t')}{\partial t} = E(q,t,q',t'), \qquad \frac{\partial S(q,t,q',t')}{\partial t'} = -E'(q,t,q',t') \tag{E.90}$$

Proof:

We first prove the second equation of (E.89) which refers to the final momemtum. We vary the final point q' while keeping the time fixed (see fig E.1). There will be a variation along the way, $\delta q(t)$, connecting the original physical motion to the new physical motion with different final position. The change in the Hamilton function δS

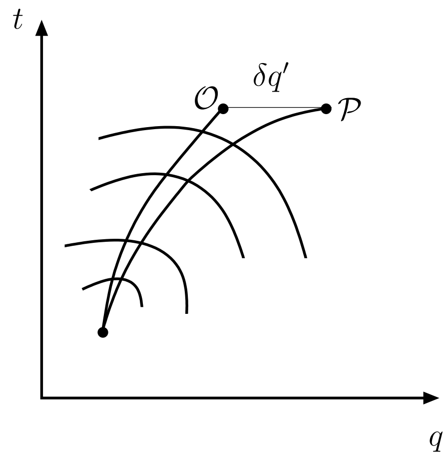

Figure E.2: Variation in the Hamilton function.

$$\begin{aligned}
\delta S &= \int_{t_0}^{t_1} \mathcal{L}(q(t)+\delta q(t), \dot{q}(t)+\delta\dot{q}(t), t)dt - \int_{t_0}^{t_1} \mathcal{L}(q(t),\dot{q}(t),t)dt \\
&= \int_{t_0}^{t_1} \left(\frac{\partial \mathcal{L}}{\partial q}\delta q + \frac{\partial \mathcal{L}}{\partial \dot{q}}\delta\dot{q} \right) dt \\
&= \int_{t_0}^{t_1} \left(\frac{\partial \mathcal{L}}{\partial q} - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}} \right) \delta q dt + \left[\frac{\partial \mathcal{L}}{\partial \dot{q}}\delta q(t) \right]_{t_0}^{t_1} \\
&= \frac{\partial \mathcal{L}}{\partial \dot{q}'}\delta q'
\end{aligned} \tag{E.91}$$

where we have put the quantity inside the parentheses of the integral to zero by the Euler-Lagrange equation. So

$$\delta S = \frac{\partial \mathcal{L}}{\partial \dot{q}'} \delta q'$$

and hence

$$\frac{\partial S}{\partial q'} = p'. \tag{E.92}$$

We first prove the second equation of (E.90) which refers to the final energy.

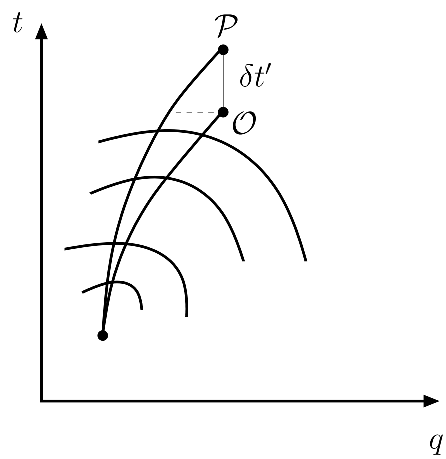

Figure E.3: Variation in the Hamilton function.

$$\begin{aligned}
\delta S &= \int_{t_0}^{t_1+\delta t} \mathcal{L}(q(t)+\delta q(t), \dot{q}(t)+\delta\dot{q}(t), t)dt - \int_{t_0}^{t_1} \mathcal{L}(q(t), \dot{q}(t), t)dt \\
&= \mathcal{L}\delta t' + \int_{t_0}^{t_1} \mathcal{L}(q(t)+\delta q(t), \dot{q}(t)+\delta\dot{q}(t), t)dt - \int_{t_0}^{t_1} \mathcal{L}(q(t), \dot{q}(t), t)dt \\
&= \mathcal{L}\delta t' + \frac{\partial \mathcal{L}}{\partial \dot{q}'} \delta q'
\end{aligned} \tag{E.93}$$

where

$$\delta q' = -\dot{q}' \delta t'$$

(see fig E.2). So

$$\delta S = \left(\mathcal{L} - \dot{q}' \frac{\partial \mathcal{L}}{\partial \dot{q}'} \right) \delta t'$$

and hence

$$\frac{\partial S}{\partial t'} = -H_0 = -E. \tag{E.94}$$

In general we have

$$\delta S = \frac{\partial \mathcal{L}}{\partial \dot{q}'}\delta q' - \left(\dot{q}'\frac{\partial \mathcal{L}}{\partial \dot{q}'} - \mathcal{L}\right)\delta t' \tag{E.95}$$

We have proved

$$\frac{\partial S}{\partial q'} = \frac{\partial \mathcal{L}(q', \dot{q}', t)}{\partial \dot{q}'} = p' \tag{E.96}$$

$$\frac{\partial S}{\partial t'} = \mathcal{L} - \dot{q}'\frac{\partial \mathcal{L}}{\partial \dot{q}'} = -H_0. \tag{E.97}$$

The Hamilton Function solves the Hamilton-Jacobi equation

Solve the first equation for $\dot{q}$ so that we have

$$\dot{q}' = \dot{q}'(q', \frac{\partial S}{\partial q'}, t')$$

and substitute the value of $\dot{q}$ into the second giving

$$\frac{\partial S}{\partial t'} + H_0\left(q', \frac{\partial S}{\partial q'}, t'\right) = 0, \tag{E.98}$$

that is, the Hamilton function solves the Hamiltonian-Jacobi equation. The Hamilton-Jacobi equation is also solved in the initial variables (q, t) in the sense that

$$-\frac{\partial S}{\partial t} + H_0\left(q, -\frac{\partial S}{\partial q}, t\right) = 0 \tag{E.99}$$

where we have a minus signs in front of the partial derivatives.

If we know the Hamilton function, we have solved the equations of motion because we obtain the general solution of the equations of motion in the form $q'(q, p, t, t')$ by simply inverting the function

$$p(q,t,q',t') = -\frac{\partial S(q,t,q',t')}{\partial q} \tag{E.100}$$

with respect to q'. The resulting function $q'(q,p,t,t')$ is the general solution of the equations of motion where the initial coordinate and momentum are q,p at time t.

Example : Free particle

The ("conventional") Hamiltonian is

$$H_0(q,p) = \frac{1}{2m}p^2. \tag{E.101}$$

From the Hamilton function (E.85)

$$S(q,t,q',t') = \frac{m(q'-q)^2}{2(t'-t)} \tag{E.102}$$

We have

$$\begin{aligned} \frac{\partial S}{\partial q'} &= m\frac{q'-q}{t'-t} = mv = p', \\ \frac{\partial S}{\partial t'} &= -\frac{m(q'-q)^2}{2(t'-t)^2} = -E' \end{aligned} \tag{E.103}$$

So that

$$\frac{\partial S}{\partial t'} + \frac{1}{2m}\left(\frac{\partial S}{\partial q'}\right)^2 = 0 \tag{E.104}$$

and therefore the Hamilton-Jacobi equation is solved.

Consider the derivative

$$\frac{\partial S}{\partial q} = -m\frac{q'-q}{t'-t} = -mv = -p. \tag{E.105}$$

Inverting this gives the general solution

$$q' = q + \frac{p}{m}(t'-t). \tag{E.106}$$

$\square$

A second example.

Example : Harmonic oscillator

The ("conventional") Hamiltonian is

$$H_0(q,p) = \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2 q^2. \tag{E.107}$$

The Hamilton function is (E.86)

$$S(q,t,q',t') = m\omega \frac{(q^2+q'^2)cos\omega(t'-t) - 2qq'}{2\sin\omega(t'-t)} \tag{E.108}$$

for motion that starts at (q,t) and ends at (q',t').

We have

$$\begin{aligned} \frac{\partial S}{\partial q'} &= m\omega\frac{q'\cos\omega(t'-t) - q}{\sin\omega(t'-t)} = mv = p', \\ \frac{\partial S}{\partial t'} &= -m\omega^2\frac{(q^2+q'^2)}{2\sin^2\omega(t'-t)} + m\omega^2\frac{qq'\cos\omega(t'-t)}{\sin^2\omega(t'-t)} = -E' \end{aligned} \tag{E.109}$$

So that

$$\begin{aligned} &\frac{\partial S}{\partial t'} + \frac{1}{2m}\left(\frac{\partial S}{\partial q'}\right)^2 + \frac{1}{2}m\omega^2 q'^2 = \\ &= -m\omega^2\frac{(q^2+q'^2)}{2\sin^2\omega(t'-t)} + m\omega^2\frac{qq'\cos\omega(t'-t)}{\sin^2\omega(t'-t)} \\ &\quad + m\omega^2\frac{q^2+q'^2\cos^2\omega(t'-t) - 2qq'\cos\omega(t'-t)}{2\sin^2\omega(t'-t)} + \frac{1}{2}m\omega^2 q'^2 \\ &= 0. \end{aligned} \tag{E.110}$$

and therefore the Hamilton-Jacobi equation is solved.

Consider the derivative

$$\frac{\partial S}{\partial q} = m\omega \frac{q \cos \omega(t' - t) - q'}{\sin \omega(t' - t)} = -p. \tag{E.111}$$

Inverting this gives the general solution

$$q' = q \cos \omega(t' - t) + \frac{p}{m\omega} \sin \omega(t' - t). \tag{E.112}$$

$\square$

E.1.7 Presympletic Formulation

A very elegant formulation of mechanics, and a crucial step in the direction of the generally covariant formulism, is provided by the presympletic formulism.

Define the covariant configuration space

$$\mathcal{C} = \mathbb{R} \times \mathcal{C}_0 \tag{E.113}$$

coordinatised by the $m+1$ variables (t, q^i).

The graph of the function $(q^i(t), p_i(t))$ is an unparametrised curve $\tilde{\gamma}$ in the $(2m+1)-$dimensional space $\Sigma = \mathbb{R}\times\Gamma_0$, with coordinates $(t, q^i(t), p_i(t))$; it is formed by all the points $(t, q^i(t), p_i(t))$ in this space. The vector field

$$X = \frac{\partial}{\partial t} + v_i(q^i, p_i)\frac{\partial f}{\partial q^i} + f_i(q^i, p_i)\frac{\partial f}{\partial p_i} \tag{E.114}$$

E.2 Generally Covariant Mechanics

The purpose of this appendix is to express dynamics in the language more wildly used, to give visual examples as well as to provide workings out. More details of ideas and physical considerations should be sought from Rovelli's book.

$$\partial_\nu = (\partial_{q^1}, \partial_{q^2} \ldots \partial_{q^m}; , \partial_{p_1}, \partial_{p_2} \ldots , \partial_{p_m}) \tag{E.115}$$

$$X^1 = \frac{\partial \mathcal{H}}{\partial q}, \;\; X^2 = \frac{\partial \mathcal{H}}{\partial p} \tag{E.116}$$

$$X_0 g = \frac{\partial \mathcal{H}}{\partial p}\frac{\partial g}{\partial q} - \frac{\partial \mathcal{H}}{\partial q}\frac{\partial g}{\partial p} \tag{E.117}$$

$$\omega_{\mu\nu} = \frac{1}{2}\left(\frac{\partial \theta_\mu}{\partial \xi^\nu} - \frac{\partial \theta_\nu}{\partial \xi^\mu}\right) \tag{E.118}$$

$$\Omega_{\mu\nu}\frac{d\xi^\nu}{ds} = -\partial_\mu f \tag{E.119}$$

$$(d\theta_0)(X_f) = -df \tag{E.120}$$

$$\Omega_{\mu\nu}\frac{d\xi^\nu}{dt} = -\partial_\mu \mathcal{H} \tag{E.121}$$

$$d\theta_0 = dx^\alpha \frac{\partial \theta_0}{\partial x^\alpha} \quad d\mathcal{H}_0 = dx^\alpha \frac{\partial \theta_0}{\partial x^\alpha} \tag{E.122}$$

$$(d\theta_0)(X) = -d\mathcal{H} \tag{E.123}$$

Presympletic

Extended phase space

$$\mathcal{C} = \mathbb{R} \times \mathcal{C}_0 \tag{E.124}$$

A simple harmonic oscillator can be viewed as a system with two partial observables, q and t A motion of the system defines a relation between q and t. A given motion is characterised by two constants $A \in [0, \infty]$ and $\phi \in [0, 2\pi]$, and is given by the equation

$$f(q,t) = q - A\sin(\omega t + \phi) = 0. \tag{E.125}$$

E.2.1 Hamiltonian Mechanics

Definition : Variational principle. A curve γ connecting the events q_1^a and q_2^a is a physical motion if $\tilde{\gamma}$ extremises the action

$$S[\tilde{\gamma}] = \int_{\tilde{\gamma}} p_a dq^a \tag{E.126}$$

in the class of curves $\tilde{\gamma}$ satisfying

$$H(q^a, p_a) = 0 \tag{E.127}$$

whose restriction γ to $\mathcal{C}$ connects q_1^a and q_2^a.

$\square$

E.2.2 Relativistic Hamilton-Jacobi Equation

$$H\left(q^a, \frac{\partial S(q^a)}{\partial q^a}\right) = 0 \tag{E.128}$$

defined on the extended configuration space $\mathcal{C}$.

E.2.3 Double Timeless Pendulum - Classical Theory

Introduction to the Double Timeless Pendulum

The Double Timeless Pendulum is a mechanical model with two partial observables, a and b. A given motion is characterised by two constants $A \in [0, \sqrt{2E}]$ and $\phi \in [0, 2\pi]$, and is given by the equation

$$f(a,b) = \left(\frac{a}{A}\right)^2 + \left(\frac{b}{B}\right)^2 - 2\frac{a}{A}\frac{b}{B}\cos\phi = \sin^2\phi. \tag{E.129}$$

Whose dynamics is defined by the relativistic Hamiltonian

$$H(a, b, p_a, p_b) = -\frac{1}{2}(p_a^2 + p_b^2 + a^2 + b^2 - 2E) = 0. \tag{E.130}$$

The Hamilton-Jacobi equation

The Hamilton-Jacobi equation is

$$\left(\frac{\partial S(a,b)}{\partial a}\right)^2 + \left(\frac{\partial S(a,b)}{\partial b}\right)^2 + a^2 + b^2 - 2E = 0. \tag{E.131}$$

We solve this using method of separation of variables. We put:

$$S(a,b) = g(a) + h(b)$$

and substitute this into (E.131),

$$\left(\frac{\partial g(a)}{\partial a}\right)^2 + a^2 = -\left(\frac{\partial h(b)}{\partial b}\right)^2 - b^2 + 2E. \tag{E.132}$$

Each side is equal to a constant, therefore we can write

$$\begin{aligned}
\left(\frac{dg(a)}{da}\right)^2 + a^2 &= A^2 \\
-\left(\frac{dh(b)}{db}\right)^2 - b^2 + 2E &= A^2.
\end{aligned} \tag{E.133}$$

The first equation becomes,

$$\frac{dg(a)}{da} = \sqrt{A^2 - a^2} \tag{E.134}$$

and so

$$g(a) = \int^a \sqrt{A^2 - \tilde{a}^2} d\tilde{a} \tag{E.135}$$

In order to arrive at the evaluation of this integral, we first write:

$$\begin{aligned}
I &= \int^a \sqrt{A^2 - \tilde{a}^2} d\tilde{a} \\
&= a\sqrt{A^2 - a^2} - \int^a \tilde{a}\frac{d}{d\tilde{a}}\left(\sqrt{A^2 - \tilde{a}^2}\right) d\tilde{a} \\
&= a\sqrt{A^2 - a^2} + \int^a \frac{\tilde{a}^2}{\sqrt{A^2 - \tilde{a}^2}} d\tilde{a} \\
&= a\sqrt{A^2 - a^2} - \int^a \frac{A^2 - \tilde{a}^2}{\sqrt{A^2 - \tilde{a}^2}} d\tilde{a} + A^2 \int^a \frac{d\tilde{a}}{\sqrt{A^2 - \tilde{a}^2}} \\
&= a\sqrt{A^2 - a^2} - I + A^2 \int^a \frac{d\tilde{a}}{\sqrt{A^2 - \tilde{a}^2}}
\end{aligned} \tag{E.136}$$

where we used integration by parts in the first step. From this we have,

$$I = \frac{a}{2}\sqrt{A^2 - a^2} + \frac{A^2}{2}\int^a \frac{d\tilde{a}}{\sqrt{A^2 - \tilde{a}^2}}. \tag{E.137}$$

To solve the integral on the RHS we use the substitution $\tilde{a} = A\sin u$,

$$\begin{aligned}
\int^a \frac{d\tilde{a}}{\sqrt{A^2 - \tilde{a}^2}} &= \int^{\arcsin(a/A)} \frac{A\cos u du}{\sqrt{A^2 - A^2\sin^2 u}} \\
&= \int^{\arcsin(a/A)} du \\
&= \arcsin\left(\frac{a}{A}\right) \\
&= \arctan\left(\frac{a}{\sqrt{A^2 - a^2}}\right).
\end{aligned} \tag{E.138}$$

Therefore

$$g(a) = \frac{a}{2}\sqrt{A^2 - a^2} + \frac{A^2}{2}\arctan\left(\frac{a}{\sqrt{A^2 - a^2}}\right). \tag{E.139}$$

The second equation, (E.133), can be written

$$\left(\frac{dh(b)}{db}\right)^2 = 2E - A^2 - b^2 \tag{E.140}$$

We immediately see that, in analogy to (E.139), that we have

$$h(b) = \frac{b}{2}\sqrt{2E - A^2 - b^2} + \frac{2E - A^2}{2}\arctan\left(\frac{b}{\sqrt{2E - A^2 - b^2}}\right). \tag{E.141}$$

So finally we have the one parameter family of solutions

$$\begin{aligned}
S(a, b, A) &= \frac{a}{2}\sqrt{A^2 - a^2} + \frac{A^2}{2}\arctan\left(\frac{a}{\sqrt{A^2 - a^2}}\right) \\
&\quad + \frac{b}{2}\sqrt{2E - A^2 - b^2} + \frac{2E - A^2}{2}\arctan\left(\frac{b}{\sqrt{2E - A^2 - b^2}}\right).
\end{aligned} \tag{E.142}$$

Derivation of the Evolution equation

The evolution equation can be obtained from

$$\frac{\partial S(a,b,A)}{\partial A} - p_A = 0. \tag{E.143}$$

We define $\phi = p_A/A$, then we have

$$\frac{\partial S(a,b,A)}{\partial A} - A\phi = 0. \tag{E.144}$$

Calculating the derivative,

$$\begin{aligned}
\frac{\partial S(a,b,A)}{\partial A} &= \frac{\partial}{\partial A}(g(a,A)+h(b,A)) \\
&= \frac{\partial}{\partial A}\int^a \sqrt{A^2-\tilde{a}^2}d\tilde{a} + \frac{\partial}{\partial A}\int^b \sqrt{2E-A^2-\tilde{b}^2}d\tilde{b} \\
&= A\int^a \frac{d\tilde{a}}{\sqrt{A^2-\tilde{a}^2}} - A\int^b \frac{d\tilde{b}}{\sqrt{2E-A^2-\tilde{b}^2}} \\
&= A\arcsin\left(\frac{a}{A}\right) - A\arcsin\left(\frac{b}{\sqrt{2E-A^2}}\right).
\end{aligned} \tag{E.145}$$

We then have

$$\arcsin\left(\frac{a}{A}\right) - \arcsin\left(\frac{b}{B}\right) = \phi. \tag{E.146}$$

where $B = \sqrt{2E-A^2}$. Using $\sin(x-y) = \sin x\cos y - \cos x \sin y$ on (E.146) gives

$$\frac{a}{A}\cos\left[\arcsin\left(\frac{b}{B}\right)\right] - \frac{b}{B}\cos\left[\arcsin\left(\frac{a}{A}\right)\right] = \sin\phi \tag{E.147}$$

Then squaring both sides gives

$$\begin{aligned}
&\left(\frac{a}{A}\right)^2\cos^2\left[\arcsin\left(\frac{b}{B}\right)\right] + \left(\frac{b}{B}\right)^2\cos^2\left[\arcsin\left(\frac{a}{A}\right)\right] \\
&-2\frac{a}{A}\frac{b}{B}\cos\left[\arcsin\left(\frac{a}{A}\right)\right]\cos\left[\arcsin\left(\frac{b}{B}\right)\right] = \sin^2\phi
\end{aligned} \tag{E.148}$$

Using $\cos^2 x = 1 - \sin^2 x$ this becomes

$$\begin{aligned}\left(\frac{a}{A}\right)^2 \left[1 - \left(\frac{b}{B}\right)^2\right] + \left(\frac{b}{B}\right)^2 \left[1 - \left(\frac{a}{A}\right)^2\right] \\ -2\frac{a}{A}\frac{b}{B} \cos\left[\arcsin\left(\frac{a}{A}\right)\right] \cos\left[\arcsin\left(\frac{b}{B}\right)\right] = \sin^2\phi.\end{aligned} \tag{E.149}$$

Using $\cos(x - y) = \cos x \cos y + \sin x \sin y$ on (E.146) we have

$$\cos\left[\arcsin\left(\frac{a}{A}\right)\right] \cos\left[\arcsin\left(\frac{b}{B}\right)\right] + \frac{a}{A}\frac{b}{B} = \cos\phi. \tag{E.150}$$

Substituting this into (E.149) gives

$$\left(\frac{a}{A}\right)^2 \left[1 - \left(\frac{b}{B}\right)^2\right] + \left(\frac{b}{B}\right)^2 \left[1 - \left(\frac{a}{A}\right)^2\right] - 2\frac{a}{A}\frac{b}{B}\left[\cos\phi - \frac{a}{A}\frac{b}{B}\right] = \sin^2\phi. \tag{E.151}$$

which easily simplifies to

$$\left(\frac{a}{A}\right)^2 + \left(\frac{b}{B}\right)^2 - 2\frac{a}{A}\frac{b}{B}\cos\phi = \sin^2\phi. \tag{E.152}$$

which is the evolution equation (E.129).

The Hamilton function

$$\begin{aligned} a' &= a'(\tau') = A\sin(\tau' + \phi) \\ b' &= b'(\tau') = B\sin(\tau') \end{aligned} \tag{E.153}$$

$$\begin{aligned} a &= a(\tau' + \tau) = A\sin(\tau' + \tau + \phi) \\ b &= b(\tau' + \tau) = B\sin(\tau' + \tau) \end{aligned} \tag{E.154}$$

We now derive the formula

$$A^2 = \frac{a^2 + a'^2 - 2aa' \cos\tau}{\sin^2\tau} \tag{E.155}$$

and

$$E = \frac{(a^2 + a'^2 + b^2 + b'^2) - 2(aa' + bb') \cos\tau}{\sin^2\tau}. \tag{E.156}$$

We first prove (E.155)

$$\begin{aligned}
&a^2 + a'^2 - 2aa' \cos\tau = \\
&= A^2\{\sin^2(\tau' + \phi + \tau) + \sin^2(\tau' + \phi) - 2\sin(\tau' + \phi + \tau)\sin(\tau' + \phi)\cos\tau\} \\
&= A^2\{[\sin(\tau' + \phi)\cos\tau + \cos(\tau' + \phi)\sin\tau]^2 + \sin^2(\tau' + \phi) \\
&\qquad -2[\sin(\tau' + \phi)\cos\tau + \cos(\tau' + \phi)\sin\tau]\sin(\tau' + \phi)\cos\tau\} \\
&= A^2\{\sin^2(\tau' + \phi)\cos^2\tau + \cos^2(\tau' + \phi)\sin^2\tau + 2\sin(\tau' + \phi)\cos\tau\cos(\tau' + \phi)\sin\tau \\
&\qquad + \sin^2(\tau' + \phi)[\cos^2\tau + \sin^2\tau] \\
&\qquad -2\sin^2(\tau' + \phi)\cos^2\tau - 2\cos(\tau' + \phi)\sin\tau\sin(\tau' + \phi)\cos\tau\} \\
&\qquad = A^2\sin^2\tau
\end{aligned} \tag{E.157}$$

giving (E.155). Similarly

$$B^2 = \frac{b^2 + b'^2 - 2aa' \cos\tau}{\sin^2\tau} \tag{E.158}$$

Therefore

$$2E = A^2 + B^2 = \frac{a^2 + a'^2 + b^2 + b'^2 - 2(aa' + bb') \cos\tau}{\sin^2\tau} \tag{E.159}$$

giving (E.156)? Rearanging gives

$$\cos^2\tau - \frac{(aa' + bb')}{E}\cos\tau + \frac{a^2 + a'^2 + b^2 + b'^2 - 2E}{2E} = 0. \tag{E.160}$$

So

$$\cos\tau = \frac{aa' + bb' + \pm\sqrt{(aa' + bb')^2 + 2E(2E - a^2 - a'^2 - b^2 - b'^2)}}{2E}. \tag{E.161}$$

and

$$\tau(a,b,a',b') = \arccos \frac{aa' + bb' + \pm\sqrt{(aa'+bb')^2 + 2E(2E - a^2 - a'^2 - b^2 - b'^2)}}{2E}. \tag{E.162}$$

E.2.4 Nonrelativistic Systems as a Special Case

E.3 Conventional Quantum Mechanics

E.3.1 Transition Amplitudes

Let $\hat{q}$ be a set of operators that commute, are complete in the sense of Dirac (form a maximally commuting set) and whose corresponding classical variables coordinatise the configuration space. Consider the basis that diagonalises these operators $\hat{q}|q >= q|q >$. The transition amplitude is then given by

$$W(q,t,q',t') = < q'|e^{-\frac{i}{\hbar}H_0(t'-t)}|q > \tag{E.163}$$

That is, the transition amplitude is given by the matrix elements of the evolution operator

$$U(t) = e^{-\frac{i}{\hbar}H_0 t} \tag{E.164}$$

in the basis $|q >$.

Notice that the transition amplitude is a function of the same variables as the Hamilton function. The transition amplitude gives the dynamics of quantum theory.

Example : Free particle For a free particle

$$W(q,t,q',t') = < q'|e^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}(t'-t)}|q > \tag{E.165}$$

Inserting the resolution of identity $\mathbf{1} = \int dp|p >< p|$,

$$\begin{aligned} W(q,t,q',t') &= \int dp \int dp' \ < q'|p' >< p'|e^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}(t'-t)}|p >< p|q > \\ &= \frac{1}{2\pi\hbar}\int dp\ e^{\frac{i}{\hbar}p(q-q') - \frac{i}{\hbar}\frac{p^2}{2m}(t'-t)} \end{aligned} \tag{E.166}$$

where we have used $< p|q >= \frac{1}{\sqrt{2\pi\hbar}} e^{ipq/\hbar}$. Evaluating the Gaussian integral we get

$$W(q,t,q',t') = A \exp \left\{ \frac{i}{\hbar} \frac{m(q'-q)^2}{2(t'-t)} \right\} \tag{E.167}$$

were the amplitude is $A = \sqrt{\frac{m}{2\pi\hbar i(t'-t)}}$. Recall that $\frac{m(q'-q)^2}{2(t'-t)}$ was the Hamilton function of this system. Therefore

$$W(q,t,q',t') \propto e^{\frac{i}{\hbar}S(q,t,q',t')}. \tag{E.168}$$

□

E.3.2 The Feynman Path Integral

The above result is general via the construction given by Feynman. Start from

$$W(q,t,q',t') = < q'|U(t'-t)|q > \tag{E.169}$$

and using the fact that the evolution operator defines a group

$$U(t'-t) = U(t'-t'')U(t''-t) \tag{E.170}$$

to write it as a product of short-time evolution operators

$$W(q,t,q',t') = < q'|U(\epsilon)\dots U(\epsilon)|q > \tag{E.171}$$

where

$$\epsilon = \frac{t'-t}{N} \tag{E.172}$$

At each step we insert the resolution of the identity

$$\mathbb{1} = \int dq_n |q_n >< q_n|. \tag{E.173}$$

The transition amplitude is then expressed by a multiple integral

$$W(q,t,q',t') = \int dq_1 \ldots dq_{N-1} \prod_{n=1}^{N} < q_n|U(\epsilon)|q_{n-1} > \qquad \text{(E.174)}$$

where we take $q = q_0$ and $q' = q_N$. This expression is true for any N. We take the limit where $N \to \infty$:

$$W(q,t,q',t') = \lim_{N\to\infty} \int dq_1 \ldots dq_{N-1} \prod_{n=1}^{N} < q_n|U(\epsilon)|q_{n-1} > . \qquad \text{(E.175)}$$

Now, consider the particular case where the Hamiltonian is of the form

$$H_0 = \frac{p^2}{2m} + V(q). \qquad \text{(E.176)}$$

The "infitesimal" evolution operator is then

$$U(\epsilon) = e^{-\frac{i}{\hbar}\left(\frac{p^2}{2m}+V(q)\right)\epsilon}. \qquad \text{(E.177)}$$

For small ϵ we can make the replacement

$$U(\epsilon) \sim e^{-\frac{i}{\hbar}\frac{p^2}{2m}\epsilon} e^{-\frac{i}{\hbar}V(q)\epsilon}, \qquad \text{(E.178)}$$

(see subsection on the Trotter product formula below). In the $|q>$ basis the second exponential gives just a number. The first was computed above in (E.166 - E.167). Together they yeild

$$\begin{aligned} < q_n|e^{-\frac{i}{\hbar}\frac{p^2}{2m}\epsilon} e^{-\frac{i}{\hbar}V(q)\epsilon}|q_{n-1} > &= < q_n|e^{-\frac{i}{\hbar}\frac{p^2}{2m}\epsilon}|q_{n-1} > e^{-\frac{i}{\hbar}V(q_n)\epsilon} \\ &= \sqrt{\frac{m}{2\pi\hbar i\epsilon}} e^{\frac{i}{\hbar}\left(\frac{m(q_n-q_{n-1})^2}{2(t_n-t_{n-1})^2}+V(q_m)\right)\epsilon} \end{aligned} \qquad \text{(E.179)}$$

The exponent in the last expression is a discretisation of the classical action. The transition amplitude can therefore be written as a multiple integral of the discretisation of the action in the limit that the discretisation is replaced by the continuous limit, namely $\epsilon \to 0$.

We then have for the tranistion amplitude

$$
\begin{aligned}
W(q,t,q',t') &= \lim_{N\to\infty}\int dq_1\ldots dq_{N-1}\prod_{n=1}^{N} < q_n|U(\epsilon)|q_{n-1}> \\
&= \lim_{N\to\infty}\left(\frac{m}{2\pi\hbar i\epsilon}\right)^{N/2}\int dq_1\ldots dq_{N-1}e^{\frac{i}{\hbar}\sum_{n=1}^{N-1}\left(\frac{m(q_n-q_{n-1})^2}{2\epsilon^2}+V(q_m)\right)\epsilon} \\
&= \lim_{N\to\infty}\mathcal{N}\int dq_1\ldots dq_{N-1}e^{\frac{i}{\hbar}S_N(q_n)}. \qquad \text{(E.180)}
\end{aligned}
$$

We now come to the reason why this object is called a "path integral" and can be seen as a "sum over histories". Imagine that the points $q, q_1, \ldots, q_{N-1}, q'$ are connected by lines. The sum in the exponential of (E.180) interpreted as a Riemann sum of a certain integral along the path - the action S.

The argument of the exponential in (E.180) is $iS/\hbar$ evaluated along the broken path connecting $q, q_1, \ldots, q_{N-1}, q'$. The integrals over the quantities $q_1, \ldots, q_{N-1}$ can be interpreted as summing over all possible broken paths connecting q and q'.

The notation for the path integral is

$$W(q,t,q',t') = \int \mathcal{D}[q(t)]e^{\frac{i}{\hbar}S[q]}. \qquad \text{(E.181)}$$

In the absence of a satifactory hamiltonian operator we can take an expression like (E.180) as a tentative ansatz for *defining* the quantum theory.

Trotter product formula

We give an outline of the argument. Putting $\lambda := i(t'-t)/\hbar$ we can write

$$W(q,t,q',t') = < q'|e^{-\lambda(T+V)/N}\ldots e^{-\lambda(T+V)/N}|q> \qquad \text{(E.182)}$$

It can be shown that

$$e^{-\lambda(T+V)/N} = e^{-\lambda T/N}e^{-\lambda V/N} + \mathcal{O}\left(\frac{\lambda^2}{N^2}\right) \qquad \text{(E.183)}$$

(worked exercie). In the limit $N\to\infty$. We wish to establish that we can replace the term

$$\left[e^{-\lambda(T+V)/N}\right]^N \qquad \text{(E.184)}$$

with the term

$$\left[e^{-\lambda T/N}e^{-\lambda V/N}\right]^N \tag{E.185}$$

We express the difference between (E.184) and (E.185) as

$$\begin{aligned}
&\left(e^{-\lambda T/N}e^{-\lambda V/N}\right)^N - \left(e^{-\lambda(T+V)/N}\right)^N \\
&\quad = \left[e^{-\lambda T/N}e^{-\lambda V/N} - e^{-\lambda(T+V)/N}\right]\left(e^{-\lambda(T+V)/N}\right)^{N-1} \\
&\quad = +e^{-\lambda T/N}e^{-\lambda V/N}\left[e^{-\lambda T/N}e^{-\lambda V/N} - e^{-\lambda(T+V)/N}\right]e^{-\lambda(T+V)^{(N-2)/N}} \\
&\quad + \cdots + \left(e^{-\lambda T/N}e^{-\lambda V/N}\right)^{N-1}\left[e^{-\lambda T/N}e^{-\lambda V/N} - e^{-\lambda(T+V)/N}\right]
\end{aligned} \tag{E.186}$$

This is an identity. It contains N terms, each of which has the factor $\exp(-\lambda T/N)\exp(-\lambda V/N) - \exp(-\lambda(T+V)/N)$, which by (E.183) is of order $1/N^2$. This justifies the replacement of (E.182) by the expression

$$W(q,t,q',t') = \lim_{N\to\infty} < q'|(e^{-\lambda T/N}e^{-\lambda V/N})^N|q > . \tag{E.187}$$

E.3.3 General Properties of Transition Amplitudes

The transition amplitude gives the wavefunction $\psi(q,t)$ given the intial wavefunction $\psi(q',t')$,

$$\psi(q',t') = \int dq\ \psi(q,t)W(q,t,q',t'). \tag{E.188}$$

The transition amplitude $W(q,t,q',t')$ is then (as a function of q') the wavefunction at time t' for a state that at time t was a delta function concentrated at q. Therefore it satisfies the Schrodinger equation in the variables (q',t') (and the conjugate equation in the variables (q,t)).

$$-i\hbar\frac{\partial}{\partial t'}W(q,t,q',t') + H_0\left(q', -i\hbar\frac{\partial}{\partial q'}\right)W(q,t,q',t') = 0. \tag{E.189}$$

Example : Free particle For a free particle

First we have

$$
\begin{aligned}
-i\hbar\frac{\partial}{\partial t'}W(q,t,q',t') &= -i\hbar\frac{\partial}{\partial t'}\left(\sqrt{\frac{m}{2\pi\hbar i(t'-t)}}\exp\left\{\frac{i}{\hbar}\frac{m(q'-q)^2}{2(t'-t)}\right\}\right) \\
&= -i\hbar\left(-\frac{1}{2(t'-t)}-\frac{i}{\hbar}\frac{m(q'-q)^2}{2(t'-t)^2}\right)W(q,t,q',t'). \quad \text{(E.190)}
\end{aligned}
$$

Then

$$
\begin{aligned}
& -H_0\left(q',-i\hbar\frac{\partial}{\partial q'}\right)W(q,t,q',t') \\
& = -A\frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial q'}\right)^2\exp\left\{\frac{i}{\hbar}\frac{m(q'-q)^2}{2(t'-t)}\right\} \\
& = \hbar^2 A\frac{1}{2m}\frac{\partial}{\partial q'}\left(\frac{i}{\hbar}\frac{m(q'-q)}{(t'-t)}\exp\left\{\frac{i}{\hbar}\frac{m(q'-q)^2}{2(t'-t)}\right\}\right) \\
= \;& \hbar^2\frac{1}{2m}\left(\frac{i}{\hbar}\frac{m}{(t'-t)}+\left(\frac{i}{\hbar}\right)^2\frac{m^2(q'-q)^2}{(t'-t)^2}\right)W(q,t,q',t') \qquad \text{(E.191)}
\end{aligned}
$$

and hence Schrodinger equation is solved. It is easy to see that $W(q,t,q',t')$ satisfies the conjugate Schrodinger equation in the variables (q,t),

$$
+i\hbar\frac{\partial}{\partial t}W(q,t,q',t')+H_0^*\left(q,-i\hbar\frac{\partial}{\partial q}\right)W(q,t,q',t')=0. \qquad \text{(E.192)}
$$

□

Example : The SHO. Normalisation factor for the SHO transition amplitude:

Use the fact that

$$
W(q,t,q',t')=A(t'-t)e^{\frac{i}{\hbar}S(q,t,q',t')} \qquad \text{(E.193)}
$$

satisfies the Schödinger equation in the variables t',q' and that $S(q,t,q',t')$ satifies the Hamilton-Jacobi equation in the variables t',q' to determine the normalisation factor $A(t'-t)$.

Solution.

The Schödinger equation in the variables t',q' is

$$-i\hbar\frac{\partial}{\partial t'}W(q,t,q',t') + \left(\frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial q'}\right)^2 + \frac{1}{2}m\omega^2 {q'}^2\right)W(q,t,q',t') = 0. \tag{E.194}$$

or

$$\begin{aligned} -i\hbar e^{\frac{i}{\hbar}S(q,t,q',t')}\frac{\partial}{\partial t'}A(t'-t) - i\hbar A(t'-t)\frac{\partial}{\partial t'}e^{\frac{i}{\hbar}S(q,t,q',t')} \\ + \left(-\frac{\hbar^2}{2m}\left(\frac{\partial}{\partial q'}\right)^2 + \frac{1}{2}m\omega^2 {q'}^2\right)W(q,t,q',t') = 0. \end{aligned} \tag{E.195}$$

This becomes

$$\begin{aligned} & i\hbar e^{\frac{i}{\hbar}S(q,t,q',t')}\frac{\partial}{\partial t'}A(t'-t) - W(q,t,q',t')\frac{\partial}{\partial t'}S(q,t,q',t') \\ &= A(t'-t)\left(-\frac{\hbar^2}{2m}\left(\frac{\partial}{\partial q'}\right)^2 + \frac{1}{2}m\omega^2 {q'}^2\right)e^{\frac{i}{\hbar}S(q,t,q',t')} \\ &= W(q,t,q',t')\left(-\frac{\hbar^2}{2m}\left(\frac{i}{\hbar}\frac{\partial^2 S}{\partial {q'}^2} - \frac{1}{\hbar^2}\left(\frac{\partial S}{\partial q'}\right)^2\right) + \frac{1}{2}m\omega^2 {q'}^2\right) \end{aligned} \tag{E.196}$$

This is greatly simplified by substitution of the Hamilton-Jacobi equation,

$$\frac{\partial S}{\partial t'} + \frac{1}{2m}\left(\frac{\partial S}{\partial q'}\right)^2 + \frac{1}{2}m\omega^2 {q'}^2 = 0 \tag{E.197}$$

to obtain

$$\frac{\partial}{\partial t'}A(t'-t) = -\frac{1}{2m}A(t'-t)\frac{\partial^2 S}{\partial {q'}^2}. \tag{E.198}$$

Now inserting the explicit expression for the Hamilton function of a harmonic oscillator, (E.86), which I reproduce here

$$S(q,t,q',t') = m\omega\frac{(q^2+{q'}^2)\cos\omega(t'-t) - 2qq'}{2\sin\omega(t'-t)} \tag{E.199}$$

for motion that starts at (q,t) and ends at (q',t'). Equation (E.198) becomes

$$\frac{\partial}{\partial t'}A(t'-t) = -\frac{1}{2}\omega A(t'-t)\cot\omega(t'-t) \tag{E.200}$$

or

$$\frac{\partial}{\partial t'}\ln A(t'-t) = -\frac{1}{2}\frac{\partial}{\partial t'}\left(\ln\sin\omega(t'-t)\right) \tag{E.201}$$

so that

$$\ln A(t'-t) = \ln C - \frac{1}{2}\left(\ln\sin\omega(t'-t)\right) \tag{E.202}$$

or

$$\begin{aligned} A(t'-t) &= C\exp\left(-\frac{1}{2}\left(\ln\sin\omega(t'-t)\right)\right) \\ &= C\sqrt{\frac{1}{\sin\omega(t'-t)}}. \end{aligned} \tag{E.203}$$

The overall constant of integration may be obtained from the free particle limit, i.e. $\omega \to 0$, of the transition amplitude which we know is

$$\sqrt{\frac{m}{2\pi\hbar i(t'-t)}}\exp\left\{\frac{i}{\hbar}\frac{m(q'-q)^2}{2(t'-t)}\right\}.$$

Therefore for the SHO we have

$$W(q,t,q',t') = \sqrt{\frac{m\omega}{2\pi\hbar i\sin\omega(t'-t)}}\exp\left\{\frac{i}{\hbar}m\omega\frac{(q^2+q'^2)\cos\omega(t'-t)-2qq'}{2\sin\omega(t'-t)}\right\} \tag{E.204}$$

□

E.4 Generally Covariant Quantum Mechanics

We have

$$< \alpha', t'| = < \alpha|e^{-iH_0 t'} \quad \text{and} \quad |\alpha, t> = e^{iH_0 t}|\alpha> \tag{E.205}$$

The propagator is defined by

$$\begin{aligned}
W(\alpha, t, \alpha', t') &= < \alpha', t'|\alpha, t> \\
&= < \alpha'|e^{-iH_0(t'-t)}|\alpha> \\
&= \sum_{mn} < \alpha'|m>< m|e^{-iH_0(t'-t)}|n>< n|\alpha> \\
&= \sum_{n} H_n(\alpha')e^{-iE_n(t'-t)}\overline{H_n(\alpha)},
\end{aligned} \tag{E.206}$$

where $H_n(\alpha)$ is the eigenfunction of H_0 with eigenvalue E_n.

E.4.1 Boundary Formalism

The probability amplitude of measuring a state ψ_t at t if the state ψ_0 was measured at time $t = 0$ is

$$A = < \psi_t|e^{-iHt}|\psi_0 > \tag{E.207}$$

Fix a time t and consider the non-relativistic boundary space

$$\mathcal{K}_t = \mathcal{H}_t^* \otimes \mathcal{H}_0 = L_2[\mathbb{R}^2, d\alpha d\alpha'] \tag{E.208}$$

where the notation $\mathcal{H}^*$ indicates the dual of the Hilbert space $\mathcal{H}$. The space $\mathcal{K}_t$ can be called a kinematic Hilbert space.

Dynamical vacuum

The linear functional W_t defined by

$$W_t\,(\psi_t \otimes \psi) := < \psi_t|e^{-iHt}|\psi_0 > \tag{E.209}$$

is well defined on $\mathcal{K}_t$. This functional captures the entire dynamics of the system. A linear functional on a Hilbert space defines a state. We denote this state $|0_t>$ defined by W_t

$$W_t(\psi) = < 0_t|\psi >_{\mathcal{K}_t} \tag{E.210}$$

and call it the "dynamical vacuum" state in boundary state space $\mathcal{K}_t$.

The states

$$|\alpha, \alpha' > = < \alpha'|_t \otimes |\alpha >_0 \tag{E.211}$$

represent a basis of the system for α at time $t = 0$ to α' at time t.

Recall

$$W(\alpha, t, \alpha', t') = < \alpha'|e^{-iH(t'-t)}|\alpha > . \tag{E.212}$$

$$\begin{aligned} < 0_t|\alpha, \alpha' > &= W_t\,(< \alpha'| \otimes |\alpha >) \\ &= < \alpha|e^{-iHt}|\alpha' > \\ &= W(\alpha, t, \alpha', 0) \end{aligned} \tag{E.213}$$

"Minkowski" vacuum

Denote $|0_M >$ the lowest eigenstate of H_0 in $\mathcal{H}_0$,

$$< \alpha|0_M > = H_0(\alpha) = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}\alpha^2} \tag{E.214}$$

Consider the analytic continuation in imaginary time of the propagator

$$W(\alpha, -it, \alpha', 0) \rightarrow_{t\rightarrow\infty} H_0(\alpha)e^{-E_0 t}\overline{H_0(\alpha')}. \tag{E.215}$$

This can be written

$$\lim_{t\rightarrow\infty} e^{E_0 t}|0_{-it} >= \ |0_M > \otimes < 0_M|. \tag{E.216}$$

This expression relates the dynamical vacuum $|0_t >$ and the Minkowski $|0_M >$. This equation can be used to find the quantum states corresponding to Minkowski spacetime from the spinfoam formulation of quantum gravity.

E.5 Conditional Probabilities

$$\mathcal{P}(a\ when\ b) = \frac{< s|\mathbb{P}\ \pi_a \pi_b \mathbb{P}|s >}{< s|\mathbb{P}\pi_b\mathbb{P}|s >} \tag{E.217}$$

E.5.1 Dolby

$$\mathcal{U}(t_{n+1}) = \mathcal{U}(t_n)\psi(t_n)$$

In order to illustrate the diffculty with this definition of probability, consider the two-state system introduced in Section 2.2, but let us imagine, for simplicity, that time is discrete. That is, the states are $\psi_S(t_n), S =\uparrow,\downarrow$ where $\psi_S(t) =< S, t_n|\psi >$, with integer n.

In the conventional formalism one focus on probabilities of the form

$$P(\uparrow \ \text{when}\ t_n),$$

where the event $(\uparrow, t_n)$ is considered as one element of the set of equal time alternatives $S_{t_n} = \{(\uparrow, t_n)(\downarrow, t_n)\}$.

But the general formalism does not privilege the time variable and therefore allows us to consider also probabilities of the form

$$\mathcal{P}(t_n\ \text{when}\ \uparrow),$$

where the event $(\uparrow, t_n)$ is considered as one element of the set of alternatives

$$S = \{\ldots, (\uparrow, t_{n-1}), (\uparrow, t_n), (\uparrow, t_{n+1}), \ldots\}.$$

$$\psi_\uparrow(t_n) = \begin{cases} 1, & \text{if } n = 1, 2 \\ 0, & \text{otherwise} \end{cases} \tag{E.218}$$

i.e.

$$\mathbb{P}\psi_\uparrow(t_n) = \psi_\uparrow(t_n)$$

then

$$
\begin{aligned}
\mathcal{P}(t_n \text{ when } \uparrow) &= \frac{< s|\pi_{t_n}\pi_\uparrow|s >}{< s|\pi_\uparrow|s >} \\
&= \sum_{s'} \frac{< s|\pi_{t_n}|s' >< s'|\pi_\uparrow|s >}{|\psi_s|^2} \\
&= \sum_{s'} \frac{< s|\pi_{t_n}|s' >< s'|\pi_\uparrow|s >}{|\psi_s|^2}
\end{aligned} \tag{E.219}
$$

where

$$
\mathcal{U}(t_0) = \mathcal{U}(t_1) = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \qquad \mathcal{U}(t_2) = \mathcal{U}(t_3) = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 1 & -1 \\ 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 \\ -1 & 1 & 0 & 0 \end{pmatrix} \tag{E.220}
$$

E.5.2 Hamilton Function of GR

$$
S_{GR}[g] = \int_{\mathcal{R}} d^n x \sqrt{\det g}\, R + \int_{\Sigma} \sqrt{\det q}\, k \tag{E.221}
$$

$$
S[q] = \int_{\Sigma} \sqrt{\det q}\, k \tag{E.222}
$$

E.6 Schrödinger Representation of Field Theory

The action for the free scalar field theory is

$$
\int d^4x\, \mathcal{L}(x) = \frac{1}{2} \int d^4x \, \left(\partial^\mu \varphi \partial_\mu \varphi - m^2 \varphi^2 \right). \tag{E.223}
$$

The conjugate field momentum is then

$$
\pi(x) = \frac{\partial \mathcal{L}}{\partial \partial_t \varphi} = \dot{\varphi}(x) \tag{E.224}
$$

The Hamiltonian density is the given in terms of the Lagrangian density via

$$\mathcal{H}_0(x) = \pi(x)\dot{\varphi}(x) - \mathcal{L}(x) \tag{E.225}$$

and so the Hamiltonian is

$$H_0 = \frac{1}{2}\int d^3x \left(\pi^2 + |\nabla\varphi|^2 + m^2\varphi^2\right). \tag{E.226}$$

We go to a coordinate Scrödinger representation and work with a basis for Fock space where the operator $\varphi(\vec{x})$, now time independent, is diagonal. Let $|\phi >$ be an eigenstate of φ with eigenvalue ϕ.

$$\varphi(\vec{x})|\phi >= \phi(\vec{x})|\phi > . \tag{E.227}$$

note $\varphi(\vec{x})$ is an operator, while $\phi(\vec{x})$ is just an ordinary scalar function.

$$\left[\frac{\delta}{\delta\phi(\vec{x})}, \phi(\vec{y})\right] = \delta(\vec{x} - \vec{y}). \tag{E.228}$$

therefore

$$\pi(\vec{x}) = -i\frac{\delta}{\delta\phi(\vec{x})} \tag{E.229}$$

in terms of the coordinate basis

$$< \phi'|\pi(\vec{x})|\phi >= -i\frac{\delta}{\delta\phi(\vec{x})}\delta(\phi - \phi'). \tag{E.230}$$

turn the Hamiltonian operator into a functional differential operator,

$$H_0 = \frac{1}{2}\int d^3x \left(-\frac{\delta^2}{\delta\phi^2(\vec{x})} + |\nabla\phi(\vec{x})|^2 + m^2\phi^2(\vec{x})\right), \tag{E.231}$$

(where $|\nabla\phi| = \partial_i\phi\partial^i\phi$) and the Schödinger

$$i\frac{\partial}{\partial t}|\Psi >= H|\Psi >, \tag{E.232}$$

turns into a functional differential equation,

$$i\frac{\partial}{\partial t}\Psi[\phi,t]=\frac{1}{2}\int d^3x\left(-\frac{\delta^2}{\delta\phi^2(\vec{x})}+|\nabla\phi|^2+m^2\phi^2\right)\Psi[\phi,t]. \tag{E.233}$$

whose solutions, the eigenfunctionals of the hamiltonian functional differential operator, represent possible states of the system. For time-independent hamiltonians it is possible to separate the variables

$$\Psi[\phi,t]=e^{-iEt}\Psi[\phi], \tag{E.234}$$

obtaining a functional eigenvalue problem for the time-independent Schödinger equation

$$\frac{1}{2}\int d^3x\left(-\frac{\delta^2}{\delta\phi^2(\vec{x})}+|\nabla\phi|^2+m^2\phi^2\right)\Psi[\phi]=E\Psi[\phi]. \tag{E.235}$$

E.6.1 Ground State and Excited States

Creation and anihilation operators can be written

$$\begin{aligned} a^\dagger(\vec{k}) &= \int d^3x e^{-i\vec{k}\cdot\vec{x}}\left(\omega_k\phi(\vec{x})-\frac{\delta}{\delta\phi(\vec{x})}\right) \\ a(\vec{k}) &= \int d^3x e^{i\vec{k}\cdot\vec{x}}\left(\omega_k\phi(\vec{x})+\frac{\delta}{\delta\phi(\vec{x})}\right). \end{aligned} \tag{E.236}$$

The Minkowski vacuum state is determined by $a\left(\vec{k}\right)|0_M>=0$. In the functional representation, this state reads

$$\Psi_{0_M}[\phi]\equiv<\phi|0_M>. \tag{E.237}$$

and is determined by

$$a\left(\vec{k}\right)\Psi_{0_M}[\phi]=\frac{\hbar}{\sqrt{2\omega}}\frac{\delta}{\delta\phi(\vec{k})}\Psi_{0_M}[\phi]+\sqrt{\frac{\omega}{2}}\phi(\vec{k})\Psi_{0_M}[\phi]=0. \tag{E.238}$$

The solution of this equation gives the functional form of the vacuum state

$$\Psi_{0_M}[\phi]=Ne^{-\frac{1}{2\hbar}\int d^3k\,\omega(\vec{k})\phi(\vec{k})\phi(\vec{k})}. \tag{E.239}$$

The one-particle state with momentum $\vec{k}$ is created by $a^\dagger(\vec{k})$:

$$\Psi_{\vec{k}}[\phi] \equiv <\phi|\vec{k}> = a^\dagger(\vec{k})\Psi_{0_M}[\phi] = \sqrt{2\omega}\phi(\vec{k})\Psi_{0_M}[\phi]. \tag{E.240}$$

It has energy $\hbar\omega(\vec{k})$. Therefore, the time-dependent state

$$\Psi_{\vec{k}}[t,\phi] = \sqrt{2\omega}e^{-i\omega(\vec{k})t}\phi(\vec{k})\Psi_{0_M}[\phi] \tag{E.241}$$

is a solution of the Wheeler-DeWitt equation

$$\left(i\hbar\frac{\partial}{\partial t} - H_0\right)\Psi = 0. \tag{E.242}$$

A generic one-particle state with wave function $f(\vec{k})$ is defined by

$$|f> \equiv \int \frac{d^3k}{\sqrt{2\omega}} f(\vec{k})|\vec{k}>, \tag{E.243}$$

and its functional representation is therefore

$$\Psi_f[\phi] \equiv <\phi|f> = \int d^3k f(\vec{k})\phi(\vec{k})\Psi_0[\phi] \tag{E.244}$$

or

$$\Psi_f[\phi] = \phi[f]\Psi_0[\phi], \tag{E.245}$$

where

$$\phi[f] = \int d^3k f(\vec{k})\phi(\vec{k}). \tag{E.246}$$

The corresponding solution to the Wheeler-DeWitt equation is

$$\Psi_f[t,\phi] = \int d^3k f(\vec{k})e^{-i\omega(\vec{k})t}\phi(\vec{k})\Psi_0[\phi] \tag{E.247}$$

as follows from

$$\left(i\hbar\frac{\partial}{\partial t} - H_0\right)\Psi_f[t,\phi] = \int \frac{d^3k}{\sqrt{2\omega}} f(\vec{k})\left(i\hbar\frac{\partial}{\partial t} - H_0\right)\sqrt{2\omega}e^{-i\omega(\vec{k})t}\phi(\vec{k})\Psi_0[\phi]$$
$$= 0. \tag{E.248}$$

or, in Fourier transform,

$$\Psi_f[t,\phi] = \int d^3x F(t,\vec{x})\phi(\vec{x})\Psi_0[\phi] \tag{E.249}$$

where

$$F(x) = F(t,\vec{x}) = \frac{1}{(2\pi)^{\frac{3}{2}}}\int d^3k e^{i(\vec{k}\cdot\vec{x}-\omega(\vec{k})t)} f(\vec{k}) \tag{E.250}$$

The $n-$(Fock)-particle state $|k_1,\ldots,k_n>$ can be obtained be repeated application of the creation operator $a^\dagger\left(\vec{k}\right)$. They have energy $\hbar(\omega_1 + \cdot + \omega_n)$ where $\omega_i(\vec{k}_i)$:

$$H_0|k_1,\ldots,k_n> = \hbar(\omega_1 + \cdot + \omega_n)|k_1,\ldots,k_n> . \tag{E.251}$$

The general solution of the Wheeler-DeWitt equation is therefore

$$\Psi[t,\phi] = \sum_n \int \frac{d^3k_1 \ldots d^3k_n}{\sqrt{2\omega_1 \ldots 2\omega_n}} f(\vec{k}_1 \ldots \vec{k}_n) e^{-i(\omega_1+\cdots+\omega_n)t}$$
$$\times a^\dagger(k_1)\ldots a^\dagger(k_n)\Psi_0[\phi]. \tag{E.252}$$

Scalar product

E.7 Transition Amplitude on an Infinite Strip

We calculate the transition amplitude for the free real massive scalar field ϕ, both in the Minkowskian space and in Euclidean space between $t_1 = 0$ and $t_2 = T$.

E.7.1 Minkowskian case

$$W_M[\varphi_1, 0, \varphi_2, T] = \int_{\varphi_1, 0, \varphi_2, T} \mathcal{D}\phi \exp\left(\frac{i}{2}\int_0^T d^4x \left(\partial_\mu \phi(x)\partial^\mu \phi(x) - m^2\phi^2\right)\right) \tag{E.253}$$

where

$$\int_0^T d^4x = \int_0^T \int_{-\infty}^{\infty} d^3x. \tag{E.254}$$

The classical equation is

$$\left(\Box_x + m^2\right)\phi(x) = 0. \tag{E.255}$$

We must now solve this equation in the infinite strip bounded by the two hyperplanes $t = 0$ and $t = T$, with boundary conditions

$$\begin{aligned} \phi(\vec{x}, 0) &= \varphi_1(\vec{x}) \\ \phi(\vec{x}, T) &= \varphi_2(\vec{x}). \end{aligned} \tag{E.256}$$

We can solve this problem by considring the Fourier transform $\tilde{\phi}(\vec{k}, t)$ of the field $\phi(\vec{x}, t)$. From equation (E.255) we have

$$\begin{aligned} \left(\Box_x + m^2\right)\phi(x) &= \int_{-\infty}^{\infty} \frac{d^3k}{(2\pi)^3}\left(\Box_x + m^2\right) e^{-i\vec{k}\cdot\vec{x}}\tilde{\phi}(\vec{k}, t) \\ &= \int_{-\infty}^{\infty} \frac{d^3k}{(2\pi)^3} e^{-i\vec{k}\cdot\vec{x}}\left(\frac{\partial^2}{\partial t^2} + \vec{k}^2 + m^2\right)\tilde{\phi}(\vec{k}, t) = 0. \end{aligned} \tag{E.257}$$

This implies

$$\left(\frac{\partial^2}{\partial t^2} + \vec{k}^2 + m^2\right)\tilde{\phi}(\vec{k}, t) = 0. \tag{E.258}$$

Solving this gives:

$$\tilde{\phi}(\vec{k}, t) = \frac{\tilde{\phi}(\vec{k}, T)\sin\omega_k t - \tilde{\phi}(\vec{k}, 0)\sin\omega_k (t - T)}{\sin\omega_k T}. \tag{E.259}$$

where $\omega_k = \sqrt{\vec{k}^2 + m^2}$ and

$$\begin{aligned}
\tilde{\phi}(\vec{k}, 0) &= \int_{-\infty}^{\infty} d^3y e^{i\vec{k}\cdot\vec{y}} \varphi_1(\vec{y}) \\
\tilde{\phi}(\vec{k}, T) &= \int_{-\infty}^{\infty} d^3y e^{i\vec{k}\cdot\vec{y}} \varphi_2(\vec{y}).
\end{aligned} \tag{E.260}$$

Putting it altogether we have

$$\overline{\phi}(x) = \int_{-\infty}^{\infty} \frac{d^3k}{(2\pi)^3} \int_{-\infty}^{\infty} d^3y e^{-\vec{k}\cdot(\vec{x}-\vec{y})} \frac{\varphi_2(\vec{y}) \sin \omega_k t - \varphi_1(\vec{y}) \sin \omega_k (t-T)}{\sin \omega_k T}. \tag{E.261}$$

Now the functional integral can be solved by substituting $\phi(x) = \overline{\phi}(x) + \eta(x)$ where $\eta(x)$ is a fluctuation:

$$\begin{aligned}
W_M[\varphi_1, 0, \varphi_2, T] &= \int_{\varphi_1, 0, \varphi_2, T} \mathcal{D}\phi \exp\left(\frac{i}{2}\int_0^T d^4x \left(\partial_\mu \phi(x) \partial^\mu \phi(x) - m^2 \phi^2\right)\right) = \\
&= \int_{\varphi_1, 0, \varphi_2, T} \mathcal{D}\phi \exp\left(\frac{i}{2}\int_0^T d^4x \left(\left(\partial_\mu \overline{\phi}(x) + \partial_\mu \eta(x)\right)^2 - m^2 \left(\overline{\phi}(x) + \eta(x)\right)^2\right)\right)
\end{aligned} \tag{E.262}$$

by using (E.255) and the boundary conditions for $\eta(x)$, namely $\eta(\vec{x}, t = 0) = 0$ and $\eta(\vec{x}, t = T) = 0$. These imply for the integral in the exponetial:

$$\begin{aligned}
&\int_0^T d^4x \left(\left(\partial_\mu \overline{\phi}(x) + \partial_\mu \eta(x)\right) \left(\partial^\mu \overline{\phi}(x) + \partial^\mu \eta(x)\right) - m^2 \left(\overline{\phi}(x) + \eta(x)\right)^2\right) = \\
&= \int_0^T d^4x \left(\partial_\mu \overline{\phi}(x) \partial^\mu \overline{\phi}(x) - m^2 \overline{\phi}^2\right) + 2\left(\partial_\mu \overline{\phi}(x) \partial^\mu \eta(x) - m^2 \overline{\phi}(x) \eta(x)\right) + \\
&\quad + \left(\partial_\mu \eta(x) \partial^\mu \eta(x) - m^2 \eta\right) \\
&= \int_0^T d^4x \left(\partial_\mu \overline{\phi}(x) \partial^\mu \overline{\phi}(x) - m^2 \overline{\phi}^2\right) - 2\left(\partial^\mu \partial_\mu \overline{\phi}(x) + m^2 \overline{\phi}(x)\right) \eta(x) + \\
&\quad + \left(\partial_\mu \eta(x) \partial^\mu \eta(x) - m^2 \eta\right) \\
&= \int_0^T d^4x \left(\partial_\mu \overline{\phi}(x) \partial^\mu \overline{\phi}(x) - m^2 \overline{\phi}^2\right) + \left(\partial_\mu \eta(x) \partial^\mu \eta(x) - m^2 \eta^2\right)
\end{aligned} \tag{E.263}$$

so that (E.262) becomes

$$W_M[\varphi_1, 0, \varphi_2, T] = \exp\left(\frac{i}{2}\int_0^T d^4x\left(\partial_\mu\overline{\phi}(x)\partial^\mu\overline{\phi}(x) - m^2\overline{\phi}^2\right)\right)$$
$$\int_{0,t=0,0,t=T}\mathcal{D}\eta\exp\left(\frac{i}{2}\int_0^T d^4x\left(\partial_\mu\eta(x)\partial^\mu\eta(x) - m^2\eta^2\right)\right) \tag{E.264}$$

Note the first term is $e^{iS_{cl}/2}$ where S_{cl} is the action evaluated for the classical field configuration $\overline{\phi}(x)$ - i.e. the Hamilton functional.

We can make a simplification:

$$\begin{aligned}
&\int_0^T d^4x\left(\partial_\mu\overline{\phi}(x)\partial^\mu\overline{\phi}(x) - m^2\overline{\phi}^2\right)\\
&= \int_0^T dx^0\int_{-\infty}^{\infty} d^3x\left(\partial_\mu[\overline{\phi}(x)\partial^\mu\overline{\phi}(x)] - \overline{\phi}(x)\partial_\mu\partial^\mu\overline{\phi}(x) - m^2\overline{\phi}^2\right)\\
&= \int_0^T dx^0\int_{-\infty}^{\infty} d^3x\left(\partial_{x^0}[\overline{\phi}(x)\partial_{x^0}\overline{\phi}(x)] - \partial_{x^i}[\overline{\phi}(x)\partial_{x^i}\overline{\phi}(x)]\right)\\
&= \int_{-\infty}^{\infty} d^3x\overline{\phi}(x)\partial_{x^0}\overline{\phi}(x)\Big|_0^T - \int_0^T dx_0\overline{\phi}(x)\partial_{x^i}\overline{\phi}(x)\Big|_{-\infty}^{\infty}\\
&= \int_{-\infty}^{\infty} d^3x\;\overline{\phi}(x)\partial_{x^0}\overline{\phi}(x)\Big|_0^T
\end{aligned} \tag{E.265}$$

where we have made use of the classical equation (E.255) again and that the field $\overline{\phi}(x)$ falls off to zero at spatial infinity. Then inserting (E.261) we have

$$\begin{aligned}
&\int_{-\infty}^{\infty} d^3x\;\overline{\phi}(x)\partial_{x^0}\overline{\phi}(x)\Big|_0^T =\\
&= \int_{-\infty}^{\infty} d^3x\int_{-\infty}^{\infty}\frac{d^3k}{(2\pi)^3}\int_{-\infty}^{\infty} d^3y e^{-\vec{k}\cdot(\vec{x}-\vec{y})}\frac{\varphi_2(\vec{y})\sin\omega_k t - \varphi_1(\vec{y})\sin\omega_k(t-T)}{\sin\omega_k T}\\
&\times\int_{-\infty}^{\infty}\frac{d^3k'}{(2\pi)^3}\int_{-\infty}^{\infty} d^3z e^{-\vec{k}'\cdot(\vec{x}-\vec{z})}\omega_{k'}\frac{\varphi_2(\vec{z})\cos\omega_{k'}t - \varphi_1(\vec{z})\cos\omega_{k'}(t-T)}{\sin\omega_{k'}T}\Big|_0^T\\
&= \int_{-\infty}^{\infty}\frac{d^3k}{(2\pi)^3}\int_{-\infty}^{\infty}\frac{d^3k'}{(2\pi)^3}\int_{-\infty}^{\infty} d^3x e^{-i\vec{x}\cdot(\vec{k}+\vec{k}')}\int_{-\infty}^{\infty} d^3y\int_{-\infty}^{\infty} d^3z e^{i\vec{k}\cdot\vec{y}}e^{i\vec{k}'\cdot\vec{z}}\omega_{k'}\\
&\left(\varphi_2(\vec{y})(\varphi_2(\vec{z})\cot\omega_{k'}T - \frac{\varphi_1(\vec{z})}{\sin\omega_{k'}T}) - \varphi_1(\vec{y})(\frac{\varphi_2(\vec{z})}{\sin\omega_{k'}T} - \varphi_1(\vec{z})\cot\omega_{k'}T)\right)\\
&= \int_{-\infty}^{\infty} d^3y\int_{-\infty}^{\infty} d^3z e^{i\vec{k}\cdot\vec{y}}\int_{-\infty}^{\infty}\frac{d^3k}{(2\pi)^3}e^{-i\vec{k}\cdot(\vec{y}-\vec{z})}\omega_k\times\\
&\times\left(-\frac{\varphi_1(\vec{y})\varphi_2(\vec{z}) + \varphi_1(\vec{z})\varphi_2(\vec{y})}{\sin\omega_k T} + \cot\omega_k T(\varphi_2(\vec{y})\varphi_2(\vec{z}) + \varphi_1(\vec{y})\varphi_1(\vec{z}))\right)
\end{aligned} \tag{E.266}$$

Now the second term in (E.264) becomes

$$\int_{0,t=0,0,t=T} \mathcal{D}\eta \exp\left(-\frac{i}{2}\int_0^T d^4x \left(\eta(x)\left(\Box_x + m^2\right)\eta(x)\right)\right) = \left(\det(-\Box - m^2)\right)^{-\frac{1}{2}}. \tag{E.267}$$

Substituting this and (E.266) into (E.264) we obtain for the transition amplitude

$$\begin{aligned} W_M[\varphi_1, 0, \varphi_2, T] \;\; = \;\; & \frac{1}{\sqrt{\det(-\Box - m^2)}} \exp\left(\frac{i}{2}\int_{-\infty}^{\infty} d^3y \int_{-\infty}^{\infty} d^3z \int_{-\infty}^{\infty} \frac{d^3k}{(2\pi)^3} e^{-i\vec{k}\cdot(\vec{y}-\vec{z})}\omega_k \right. \\ & \left.\left(-\frac{\varphi_1(\vec{y})\varphi_2(\vec{z}) + \varphi_1(\vec{z})\varphi_2(\vec{y})}{\sin\omega_k T} + \cot\omega_k T(\varphi_2(\vec{y})\varphi_2(\vec{z}) + \varphi_1(\vec{y})\varphi_1(\vec{z}))\right)\right). \end{aligned} \tag{E.268}$$

The inifinite factor $(\det(-\Box - m^2))^{-\frac{1}{2}}$ will be dealt with in a later subsection.

E.7.2 Euclidean case

We now explicitly calculate the transition amplitude for a free massive scalar field in euclidean space, using a slightly different method that will be used again in the calculation of the generalised Tomonaga-Schwinger equation.

$$W_E[\varphi_1, 0, \varphi_2, T] = \int_{\varphi_1,0,\varphi_2,T} \mathcal{D}\phi \exp\left(-\frac{1}{2}\int_0^T d^4x \left(\partial_\mu\phi(x)\partial^\mu\phi(x) + m^2\phi^2\right)\right) \tag{E.269}$$

classical equation

$$\left(\Box_x - m^2\right)\phi(x) = 0. \tag{E.270}$$

We now solve this equation using the Green function technique. The Green's function satisfies the equation

$$\left(\Box_x - m^2\right)G(x, y) = -\delta^4(x - y). \tag{E.271}$$

This can be rewritten as

$$\int_0^T d^4x \left(G(x,y)\left(\Box_x - m^2\right)\overline{\phi}(x) - \overline{\phi}(x)\left(\Box_x - m^2\right)G(x,y)\right) =$$
$$= \int_0^T d^4x\delta^4(x-y)\overline{\phi}(x) \tag{E.272}$$

that is

$$\begin{aligned}
\overline{\phi}(y) &= \int_0^T d^4x \left(G(x,y)\Box_x\overline{\phi}(x) - \overline{\phi}(x)\Box_x G(x,y)\right) \\
&= \int_0^T dx^0 \int_{-\infty}^{\infty} d^3x \left(G(x,y)\partial^2_{x^i}\overline{\phi}(x) - \overline{\phi}(x)\partial^2_{x^i}G(x,y) + \right. \\
&\qquad \left. + G(x,y)\partial^2_{x^0}\overline{\phi}(x) - \overline{\phi}(x)\partial^2_{x^0}G(x,y)\right) \\
&= \int_0^T dx^0 \int_{-\infty}^{\infty} d^3x \left[\partial_{x^i}\left(G(x,y)\partial_{x^i}\overline{\phi}(x) - \overline{\phi}(x)\partial_{x^i}G(x,y)\right) + \right. \\
&\qquad \left. + \partial_{x^0}\left(G(x,y)\partial_{x^0}\overline{\phi}(x) - \overline{\phi}(x)\partial_{x^0}G(x,y)\right)\right] \\
&= \int_0^T dx^0 \int_{-\infty}^{\infty} d^3x \left[\partial_{x^i}\left(G(x,y)\overleftrightarrow{\partial}_{x^i}\overline{\phi}(x)\right) + \partial_{x^0}\left(G(x,y)\overleftrightarrow{\partial}_{x^0}\overline{\phi}(x)\right)\right]
\end{aligned} \tag{E.273}$$

where $G \overleftrightarrow{\partial} \phi = G\partial\phi - \phi\partial G$. Supposing that $G(x,y)$ and $\phi(x)$ go to zero fast enough at spatial infinity the first term of the sum is zero, and so

$$\begin{aligned}
\overline{\phi}(y) &= \int_{-\infty}^{\infty} d^3x \int_0^T dx^0\partial_{x^0}\left(G(x,y)\overleftrightarrow{\partial}_{x^0}\overline{\phi}(x)\right) \\
&= \int_{-\infty}^{\infty} d^3x \left[G(x,y)\overleftrightarrow{\partial}_{x^0}\overline{\phi}(x)\right]_{x^0=0}^{x^0=T} \\
&= \int_{-\infty}^{\infty} d^3x \left[G(\vec{x},T,y)\,\partial_{x^0}\overline{\phi}(x)\big|_{x^0=T} - \partial_{x^0}G(x,y)\big|_{x^0=T}\,\varphi_2(\vec{x}) + \right. \\
&\quad \left. - G(\vec{x},0,y)\,\partial_{x^0}\overline{\phi}(x)\big|_{x^0=0} + \partial_{x^0}G(x,y)\big|_{x^0=0}\,\varphi_1(\vec{x})\right]
\end{aligned} \tag{E.274}$$

To reproduce the boundary conditions $\phi(\vec{x},0) = \varphi_1(\vec{x})$ and $\phi(\vec{x},T) = \varphi_2(\vec{x})$ the Green function G must be zero for $x_0 = 0$ and $x_0 = T$. Then

$$\overline{\phi}(y) = \int_{-\infty}^{\infty} d^3x \left(\partial_{x^0}G(\vec{x},0,y)\,\varphi_1(\vec{x}) - \partial_{x^0}G(\vec{x},T,y)\,\varphi_2(\vec{x})\right). \tag{E.275}$$

We solve (E.271) with a "spatial" Fourier transform:

$$\begin{aligned}
G(x,y) &= \int \frac{d^3k}{(2\pi)^3}\tilde{G}(x_0,y_0)e^{-i(\vec{x}-\vec{y})} \\
\delta^4(x-y) &= \int \frac{d^3k}{(2\pi)^3}\delta(x_0-y_0)e^{-i(\vec{x}-\vec{y})}
\end{aligned} \tag{E.276}$$

imposing the conditions

$$\tilde{G}(0,y_0) = \tilde{G}(t,y_0) = 0. \tag{E.277}$$

Employing (E.276) in (E.271) we have:

$$\int \frac{d^3k}{(2\pi)^3}\left(\Box_x - m^2\right)\tilde{G}(x_0,y_0)e^{-i(\vec{x}-\vec{y})} = -\int \frac{d^k}{(2\pi)^3}\delta(x_0-y_0)e^{-i(\vec{x}-\vec{y})}. \tag{E.278}$$

Which gives

$$\left(\partial^2_{x_0} - (\vec{k}^2+m^2)\right)\tilde{G}(x_0,y_0) = -\delta(x_0-y_0). \tag{E.279}$$

The general solution is of the form

$$\tilde{G}(x_0,y_0) = \tilde{G}_p(x_0,y_0) + \left[A(\vec{k},y_0)f_1(\vec{k},x_0) + B(\vec{k},y_0)f_2(\vec{k},x_0)\right] \tag{E.280}$$

where $\tilde{G}_p(x_0,y_0)$ is a solution (i.e., any solution) of the inhomogeneous equation and $f_1(\vec{k},x_0)$, $f_2(\vec{k},x_0)$ are two linearly independent solutions of the homogeneous equation. The homogeneous solutions are helpful in obtaing the correct boundary conditions.

A solution of the inhomogeneous equation is

$$\frac{1}{2\omega_k}e^{-\omega_k|x_0-y_0|}. \tag{E.281}$$

We check this,

$$\begin{aligned}
\partial^2_{x_0}\left[\frac{1}{2\omega_k}e^{-\omega_k|x_0-y_0|}\right] &= \partial_{x_0}\left[-\omega_k\left(2\Theta(x_0-y_0)-1\right)\frac{1}{2\omega_k}e^{-\omega_k|x_0-y_0|}\right] \\
&= \left(-\delta(x_0-y_0) + \omega_k^2\frac{1}{2\omega_k}e^{-\omega_k|x_0-y_0|}\right),
\end{aligned}$$

which rearranged gives

$$\left(\partial_{x_0}^2 - (\vec{k}^2 + m^2)\right) \frac{1}{2\omega_k} e^{-\omega_k |x_0 - y_0|} = -\delta(x_0 - y_0). \tag{E.282}$$

Two linearly independent homogeneous solutions are obviously $e^{\omega_k x_0}$ and $e^{-\omega_k x_0}$. Therefore

$$\tilde{G}(x_0, y_0) = \frac{1}{2\omega_k} e^{-\omega_k |x_0 - y_0|} + A(\vec{k}, y_0) e^{\omega_k x_0} + B(\vec{k}, y_0) e^{-\omega_k x_0}. \tag{E.283}$$

We now impose the boundary conditions (E.277)

$$\begin{aligned} \tilde{G}(0, y_0) &= \frac{1}{2\omega_k} e^{-\omega_k y_0} + A(\vec{k}, y_0) + B(\vec{k}, y_0) = 0 \\ \tilde{G}(T, y_0) &= \frac{1}{2\omega_k} e^{-\omega_k (T - y_0)} + A(\vec{k}, y_0) e^{\omega_k T} + B(\vec{k}, y_0) e^{-\omega_k T} = 0 \end{aligned} \tag{E.284}$$

which are solved by appropriate choices for $A(\vec{k}, y_0)$ and $B(\vec{k}, y_0)$. From these equations we obtain

$$\tilde{G}(T, y_0) - \tilde{G}(0, y_0) e^{-\omega_k T} = \frac{1}{2\omega_k} e^{-\omega_k (T - y_0)} - \frac{1}{2\omega_k} e^{-\omega_k y_0} e^{-\omega_k T} + A(\vec{k}, y_0)(e^{\omega_k T} - e^{-\omega_k T}) = 0 \tag{E.285}$$

and

$$\tilde{G}(0, y_0) e^{\omega_k T} - \tilde{G}(T, y_0) = \frac{1}{2\omega_k} e^{-\omega_k y_0} e^{\omega_k T} - \frac{1}{2\omega_k} e^{-\omega_k (T - y_0)} + B(\vec{k}, y_0)(e^{\omega_k T} - e^{-\omega_k T}) = 0 \tag{E.286}$$

so that

$$A(\vec{k}, y_0) = \frac{e^{-\omega_k y_0} e^{-\omega_k T} - e^{-\omega_k (T - y_0)}}{2\omega_k (e^{\omega_k T} - e^{-\omega_k T})} \tag{E.287}$$

$$B(\vec{k}, y_0) = \frac{e^{-\omega_k (T - y_0)} - e^{-\omega_k y_0} e^{\omega_k T}}{2\omega_k (e^{\omega_k T} - e^{-\omega_k T})} \tag{E.288}$$

Substituting these into (E.283), and expressing $G(x,y)$ as the "spatial" Fourier transformation, we finally have for the Green function $G(x,y)$:

$$
\begin{aligned}
G(x,y) &= \int \frac{d^3k}{(2\pi)^3} e^{-i\vec{k}\cdot(\vec{x}-\vec{y})} \left(\frac{1}{2\omega_k} e^{-\omega_k|x_0-y_0|} + \right. \\
& \left. + \frac{e^{-\omega_k y_0} e^{-\omega_k T} - e^{-\omega_k(T-y_0)}}{2\omega_k(e^{\omega_k T} - e^{-\omega_k T})} e^{\omega_k x_0} + \frac{e^{-\omega_k(T-y_0)} - e^{-\omega_k y_0} e^{\omega_k T}}{2\omega_k(e^{\omega_k T} - e^{-\omega_k T})} e^{-\omega_k x_0} \right).
\end{aligned}
\tag{E.289}
$$

We now wish to substitute this into (E.275). First we calculate

$$
\begin{aligned}
\partial_{x^0} \tilde{G}(x_0, y_0) &= -\frac{1}{2}(2\Theta(x_0 - y_0) - 1) e^{-\omega_k|x_0-y_0|} + \\
& + e^{-\omega_k y_0} \frac{e^{\omega_k T} e^{-\omega_k x_0} + e^{-\omega_k T} e^{\omega_k x_0}}{2(e^{\omega_k T} - e^{-\omega_k T})} \\
& - e^{\omega_k y_0} \frac{e^{\omega_k x_0} + e^{-\omega_k x_0}}{2(e^{\omega_k T} - e^{-\omega_k T})} e^{-\omega_k T}
\end{aligned}
\tag{E.290}
$$

Then

$$
\begin{aligned}
\partial_{x^0} \tilde{G}(0, y_0) &= \frac{1}{2} e^{-\omega_k y_0} + \frac{1}{2} e^{-\omega_k y_0} \frac{\cosh \omega_k T}{\sinh \omega_k T} - \frac{1}{2} e^{\omega_k y_0} \frac{e^{-\omega_k T}}{\sinh \omega_k T} \\
&= -\frac{\sinh \omega_k (y_0 - T)}{\sinh \omega_k T}
\end{aligned}
\tag{E.291}
$$

and

$$
\begin{aligned}
\partial_{x^0} \tilde{G}(T, y_0) &= -\frac{1}{2} e^{-\omega_k(T-y_0)} + \frac{1}{2} e^{-\omega_k y_0} \frac{1}{\sinh \omega_k T} - \frac{1}{2} e^{-\omega_k(T-y_0)} \frac{\cosh \omega_k T}{\sinh \omega_k T} \\
&= +\frac{1}{2} e^{-\omega_k y_0} \frac{1}{\sinh \omega_k T} - \frac{1}{2} e^{-\omega_k(T-y_0)} \frac{1}{\sinh \omega_k T} e^{\omega_k T} \\
&= -\frac{\sinh \omega_k y_0}{\sinh \omega_k T}
\end{aligned}
\tag{E.292}
$$

substituting this into (E.275), the formula that we repeat here

$$\overline{\phi}(y) = \int_{-\infty}^{\infty} d^3x \int \frac{d^3k}{(2\pi)^3} e^{-i\vec{k}\cdot(\vec{x}-\vec{y})} \left(\partial_{x^0}\tilde{G}(0,y_0)\ \varphi_1(\vec{x}) - \partial_{x^0}\tilde{G}(T,y_0)\ \varphi_2(\vec{x})\right) \tag{E.293}$$

we have

$$\overline{\phi}(x) = \int_{-\infty}^{\infty} d^3y \int \frac{d^3k}{(2\pi)^3} e^{-i\vec{k}\cdot(\vec{x}-\vec{y})} \frac{\sinh\omega_k t\ \varphi_2(\vec{y}) - \sinh\omega_k(t-T)\varphi_1(\vec{y})}{\sinh\omega_k T}. \tag{E.294}$$

The functional integral can be soved exactly as in the minkowskian case, to obtain

$$\begin{aligned} W_E[\varphi_1, 0, \varphi_2, T] \quad = \quad & \frac{1}{\sqrt{\det(-\Box - m^2)}} \exp\left(-\frac{1}{2}\int_{-\infty}^{\infty} d^3y \int_{-\infty}^{\infty} d^3z \int_{-\infty}^{\infty} \frac{d^3k}{(2\pi)^3} e^{-i\vec{k}\cdot(\vec{y}-\vec{z})}\omega_k \right. \\ & \left.\left(-\frac{\varphi_1(\vec{y})\varphi_2(\vec{z}) + \varphi_1(\vec{z})\varphi_2(\vec{y})}{\sinh\omega_k T} + \coth\omega_k T(\varphi_2(\vec{y})\varphi_2(\vec{z}) + \varphi_1(\vec{y})\varphi_1(\vec{z}))\right)\right). \end{aligned} \tag{E.295}$$

E.7.3 Normalisation Factor

Minkowskian case

To find the correct normaqlisation factor for the transition amplitude, we sue that it satify the functional Schrödinger equation

$$i\frac{\partial}{\partial T} W_M[\varphi_1, 0, \varphi_2, 0, T] = \frac{1}{2}\left(-\frac{\delta^2}{\delta\varphi_2^2(\vec{x})} + |\nabla\varphi_2(\vec{x})|^2 + m^2\varphi_2^2(\vec{x})\right) W_M[\varphi_1, 0, \varphi_2, 0, T] \tag{E.296}$$

By writing the transition amplitude as $W_M[\varphi_1, 0, \varphi_2, 0, T] = M(T)\exp\left(iS[\varphi_1, \varphi_2]\right)$, (E.296) reads as

$$\begin{aligned} i\exp\left(iS[\varphi_1,\varphi_2]\right)\frac{\partial}{\partial T}M(T) - W_M[\varphi_1, 0, \varphi_2, T]\frac{\partial}{\partial T}S[\varphi_1,\varphi_2] = W_M[\varphi_1, 0, \varphi_2, 0, T]\cdot \\ \cdot\frac{1}{2}\int d^3x \left(\left(-i\frac{\delta^2 S[\varphi_1,\varphi_2]}{\delta\varphi_2^2(\vec{x})} + \left(\frac{\delta S[\varphi_1,\varphi_2]}{\delta\varphi_2(\vec{x})}\right)^2\right) + \left(|\nabla\varphi_2(\vec{x})|^2 + m^2\varphi_2^2(\vec{x})\right)\right) \end{aligned} \tag{E.297}$$

This is greatly simplified by substitution of the Hamilton-Jacobi equation, that is, the classical action calculated on the boundary conditions, and as such obeys

$$\begin{aligned} 0 &= \frac{\partial S}{\partial T} + H_0\left(\varphi_2, \frac{\delta S}{\delta \varphi_2}\right) \\ &= \frac{\partial S}{\partial T} + \frac{1}{2}\int d^3x \left(\left(\frac{\delta S}{\delta \varphi_2}\right)^2 + |\nabla \varphi_2(\vec{x})|^2 + m^2\varphi_2^2(\vec{x})\right), \end{aligned} \tag{E.298}$$

to obtain

$$i\exp\left(iS[\varphi_1,\varphi_2]\right)\frac{\partial}{\partial T}M(T) = -\frac{i}{2}W_M[\varphi_1, 0, \varphi_2, 0, T]\int d^3x \frac{\delta^2 S[\varphi_1,\varphi_2]}{\delta\varphi_2^2(\vec{x})}. \tag{E.299}$$

From the exponent of (E.268),

$$\begin{aligned} S[\varphi_1,\varphi_2] &= \frac{1}{2}\int_{-\infty}^{\infty} d^3y \int_{-\infty}^{\infty} d^3z \int_{-\infty}^{\infty} \frac{d^3k}{(2\pi)^3} e^{-i\vec{k}\cdot(\vec{y}-\vec{z})}\omega_k \\ &\left(-\frac{\varphi_1(\vec{y})\varphi_2(\vec{z}) + \varphi_1(\vec{z})\varphi_2(\vec{y})}{\sin\omega_k T} + \cot\omega_k T(\varphi_2(\vec{y})\varphi_2(\vec{z}) + \varphi_1(\vec{y})\varphi_1(\vec{z}))\right) \end{aligned} \tag{E.300}$$

we obtain

$$\begin{aligned} \int d^3x \frac{\delta^2 S[\varphi_1,\varphi_2]}{\delta\varphi_2^2(\vec{x})} &= \int d^3x \frac{1}{2}\int_{-\infty}^{\infty} d^3y \int_{-\infty}^{\infty} d^3z \int_{-\infty}^{\infty} \frac{d^3k}{(2\pi)^3} e^{-i\vec{k}\cdot(\vec{y}-\vec{z})} \\ &\quad \cot\omega_k T(2\delta(\vec{x}-\vec{y})\delta(\vec{x}-\vec{z})) \\ &= V\int_{-\infty}^{\infty} \frac{d^3k}{(2\pi)^3}\omega_k \cot\omega_k T. \end{aligned} \tag{E.301}$$

where V is a volume. Substituting this into (E.299) we get

$$\frac{\partial}{\partial T}M(T) = -\frac{1}{2}M(T)V\int_{-\infty}^{\infty}\frac{d^3k}{(2\pi)^3}\omega_k \cot\omega_k T \tag{E.302}$$

or

$$\frac{\partial}{\partial T}\ln M(T) = -\frac{1}{2}V\frac{\partial}{\partial T}\int_{-\infty}^{\infty}\frac{d^3k}{(2\pi)^3}\omega_k \ln\sin\omega_k T \tag{E.303}$$

so that

$$M(T) = C \exp\left(-\frac{1}{2}V\int_{-\infty}^{\infty}\frac{d^3k}{(2\pi)^3}\omega_k \ln\sin\omega_k T\right). \tag{E.304}$$

E.7.4 Relation to the Vacuum State

Minkowski vacuum

$$\Psi_0[\phi] = \exp\left(-\frac{1}{2}\int d^3y\int d^3z\int\frac{d^3p}{(2\pi)^3}e^{i\vec{p}\cdot(\vec{y}-\vec{z})}\sqrt{\vec{p}^2+m^2}\psi(\vec{z})\psi(\vec{y})\right) \tag{E.305}$$

This functional corresponds to the vacuum state defined as the state with the lowest energy. In the following we call the Minkowski vacuum the vacuum state defined this way, to distinguish it from another vacuum state that will be defined shortly.

Choose a basis $|n>$ of eigenstates of H_0 with eigenvalues E_n, and consider the operator

$$W(T) = \sum_n e^{-TE_n}|n><n|. \tag{E.306}$$

In the large T limit, this becomes the projector on the vacuum

$$\lim_{T\to\infty} W(T) = |0_M><0_M|. \tag{E.307}$$

Nonperturbative vacuum

We define a kinematic Hilbert space $\mathcal{K}_{\Sigma_T}$, as the tensor product

$$\mathcal{K}_{\Sigma_T} := \mathcal{H}^*_{t=T}\otimes\mathcal{H}_{t=0} \tag{E.308}$$

where the notation $\mathcal{H}^*$ indicates the dual of the Hilbert space $\mathcal{H}$; which of course is canonically isomorphic to $\mathcal{H}$. We denote a field on Σ_T by $\phi = (\varphi_1, \varphi_2)$. The field basis of the Fock space induces in $\mathcal{K}_{\Sigma_T}$ the basis

$$|\phi>=|\varphi_1,\varphi_2> = <\varphi_2|_{t=T}\otimes|\varphi_1>_{t=0}, \tag{E.309}$$

which in the language of wave functionals translates as

$$\Psi[\phi] = \Psi[\varphi_1, \varphi_2] = < \varphi_1, \varphi_2 | \Psi > . \tag{E.310}$$

In the kinematic Hilbert space $\mathcal{K}_{\Sigma_T}$ the transition amplitude $W[\varphi_1, 0; \varphi_2, T]$ defines a preferred (bra) state

$$< 0_{\mathcal{K}_{\Sigma_T}} | \Psi > = W[\varphi_1, 0; \varphi_2, T] \tag{E.311}$$

is this Hilbert space. The state is referred to as the *nonperturbative vacuum*, or covariant vacuum. This state expresses the dynamics from $t = 0$ to $t = T$. As a state in $\mathcal{K}_{\Sigma_T}$, which is the tensor product of two Hilbert spaces, it defines a linear mapping between the two spaces $\mathcal{H}_{t=0}$ and $\mathcal{H}_{t=T}$. The linear mapping is precisely the (imaginary time) evolution e^{-TH}. We have by construction

$$< 0_{\mathcal{K}_{\Sigma_T}} | \, (< \psi_{out} | \otimes | \psi_{in} >) = < \psi_{out} | e^{-TH} | \psi_{in} > . \tag{E.312}$$

Or

$$< 0_{\mathcal{K}_{\Sigma_T}} | \psi_{in} >= e^{-TH} | \psi_{in} > . \tag{E.313}$$

Notice that the bra/ket mismatch is apparent only, as the three states live in different Hilbert spaces.

Equation (E.306) shows that in the limit $T \to \infty$ we have the projector on the vacuum

$$\lim_{T \to \infty} < 0_{\mathcal{K}_{\Sigma_T}} | \, (< \psi_{out} | \otimes | \psi_{in} >) = < \psi_{out} | 0_M > \; < 0_M | \psi_{in} > . \tag{E.314}$$

We can therefore write the relation the two notions of vacuum that we have defined as

$$\lim_{T \to \infty} | 0_{\mathcal{K}_{\Sigma_T}} > = | 0_M > \otimes < 0_M |. \tag{E.315}$$

E.8 General Boundary Formulation

E.9 Generalised Schödinger Equation in Euclidean Field Theory

E.9.1 Surfaces and Surface Derivatives

Consider a finite region $\mathcal{R}$ in the euclidean $4d$ space $\mathbb{R}^4$. we use cartesian coordinates $x, y, z, \ldots$ on $\mathbb{R}^4$ where $x = (x^a)$, $a = 1, 2, 3, 4$. Let $\Sigma = \partial \mathcal{R}_\Sigma$ be a compact 3d surface that bounds a finite region $\mathcal{R}_\Sigma$. We denote $s, t, u \ldots$ coordinates on Σ, where $s = (s^q)$, $q = 1, 2, 3$.

A line element is given by

$$d\tau^2 = q_{qr}(s) ds^q ds^r = g_{ab} \left(\frac{\partial x^a}{\partial s^q} ds^q \right) \left(\frac{\partial x^b}{\partial s^q} ds^r \right) \tag{E.316}$$

the induced metric is then

$$q_{ab}(s) = \frac{\partial x^a(s)}{\partial s^q} \frac{\partial x_a(s)}{\partial s^r} \tag{E.317}$$

The surface gradient is defined as

$$\nabla^q := \frac{\partial}{\partial s^q} \tag{E.318}$$

The normal one-form of the surface is

$$\tilde{n}_a(s) = \epsilon_{abcd} \frac{\partial x^b(s)}{\partial s^1} \frac{\partial x^c(s)}{\partial s^2} \frac{\partial x^d(s)}{\partial s^3}. \tag{E.319}$$

We orient the coordinate system s so that $\tilde{n}_a$ is outward directed. Its norm is easily seen to be the determinate of the induced metric q_{qr}, (see append on measurement of area),

$$\tilde{n}_a \tilde{n}^a = \det q. \tag{E.320}$$

Proof.

$$
\begin{aligned}
\tilde{n}^a \tilde{n}_a &= \epsilon^{abcd}\epsilon_{ab'c'd'} \frac{\partial x_b(s)}{\partial s^1}\frac{\partial x_c(s)}{\partial s^2}\frac{\partial x_d(s)}{\partial s^3}\frac{\partial x^{b'}(s)}{\partial s^1}\frac{\partial x^{c'}(s)}{\partial s^2}\frac{\partial x^{d'}(s)}{\partial s^3} \\
&= \delta^{bcd}_{b'c'd'} \frac{\partial x_b(s)}{\partial s^1}\frac{\partial x_c(s)}{\partial s^2}\frac{\partial x_d(s)}{\partial s^3}\frac{\partial x^{b'}(s)}{\partial s^1}\frac{\partial x^{c'}(s)}{\partial s^2}\frac{\partial x^{d'}(s)}{\partial s^3} \\
&= \det \begin{pmatrix} \delta^b_{b'} & \delta^c_{b'} & \delta^d_{b'} \\ \delta^b_{c'} & \delta^c_{c'} & \delta^d_{c'} \\ \delta^b_{d'} & \delta^c_{d'} & \delta^d_{d'} \end{pmatrix} \frac{\partial x_b(s)}{\partial s^1}\frac{\partial x_c(s)}{\partial s^2}\frac{\partial x_d(s)}{\partial s^3}\frac{\partial x^{b'}(s)}{\partial s^1}\frac{\partial x^{c'}(s)}{\partial s^2}\frac{\partial x^{d'}(s)}{\partial s^3} \\
&= \det \begin{pmatrix} \frac{\partial x_b(s)}{\partial s^1}\frac{\partial x^b(s)}{\partial s^1} & \frac{\partial x_b(s)}{\partial s^1}\frac{\partial x^b(s)}{\partial s^2} & \frac{\partial x_b(s)}{\partial s^1}\frac{\partial x^b(s)}{\partial s^3} \\ \frac{\partial x_b(s)}{\partial s^2}\frac{\partial x^b(s)}{\partial s^1} & \frac{\partial x_b(s)}{\partial s^2}\frac{\partial x^b(s)}{\partial s^2} & \frac{\partial x_b(s)}{\partial s^2}\frac{\partial x^b(s)}{\partial s^3} \\ \frac{\partial x_b(s)}{\partial s^3}\frac{\partial x^b(s)}{\partial s^1} & \frac{\partial x_b(s)}{\partial s^3}\frac{\partial x^b(s)}{\partial s^2} & \frac{\partial x_b(s)}{\partial s^3}\frac{\partial x^b(s)}{\partial s^3} \end{pmatrix} \\
&= \det \begin{pmatrix} q_{11}(s) & q_{12}(s) & q_{13}(s) \\ q_{21}(s) & q_{22}(s) & q_{23}(s) \\ q_{31}(s) & q_{32}(s) & q_{33}(s) \end{pmatrix} \\
&= \det q(s)
\end{aligned}
\tag{E.321}
$$

where we have used (E.317).

In the following we use the normalised normal

$$
n_a \equiv (\det q)^{-\frac{1}{2}}\, \tilde{n}_a \tag{E.322}
$$

and the induced volume element on Σ

$$
d\Sigma(s) \equiv (\det q)^{\frac{1}{2}}\ d^3 s. \tag{E.323}
$$

Given a functional $F[\Sigma]$ that depends on the surface, we define the functional deriviative with respect to the surface as the normal projection of the functional derivative with respect to the embedding that defines the surface

$$
\frac{\delta}{\delta\Sigma(s)} \equiv n^a(s)\frac{\delta}{\delta x^a(s)} \tag{E.324}
$$

Here the functional derivative on the right hand side is defined in terms of the volume element $d\Sigma$.

$$
\int d\Sigma(s) N(s) \frac{\delta F[\Sigma]}{\delta\Sigma(s)} = \int d\Sigma N(s)\frac{\delta F[\Sigma]}{\delta x^a(s)} n^a(s) = \lim_{\epsilon\to 0}\frac{F[\Sigma_{\epsilon N}] - F[\Sigma]}{\epsilon} \tag{E.325}
$$

where $\Sigma_{\epsilon N}$ is the deformed surface defined by

$$x^a(s) + \epsilon N(s) n^a(s). \tag{E.326}$$

$$F_f[\Sigma] := \int_{\mathcal{R}} d^4x f(x) \tag{E.327}$$

Then

$$\frac{\delta F_f[\Sigma]}{\delta \Sigma(s)} = f(x(s)). \tag{E.328}$$

That is, the variation of the bulk integral under normal variation of the surface is the integrand in the variation point.

E.10 Relation to the Vacuum State

corresponds to the state with the lowest energy.

E.11 Generalised Tomonaga-Swinger Equation

It was demonstrated that $W[\varphi, \Sigma]$ satisfies a local functional equation governing the variation of $W[\varphi, \Sigma]$ under arbitrary local deformations of Σ, namely

$$\frac{\delta W[\varphi, \Sigma]}{\delta \Sigma(s)} = H_0 \left(\varphi(s), \nabla \varphi(s), \frac{\delta}{\delta \varphi(s)} \right) W[\varphi, \Sigma] \tag{E.329}$$

Equation (E.329) was derived on the basis of a lattice regularisation of the functional integral

$$W[\varphi, \Sigma] = \int_{\phi|_\Sigma = \varphi} \mathcal{D}\phi e^{-S[\phi]} \tag{E.330}$$

defining $W[\varphi, \Sigma]$, and under certain hypotheses on the existence of the continuum limit. In this section, working in context of the free euclidean theory, we show that this equation can be derived from the functional integral definition of $W[\varphi, \Sigma]$ directly in the continuum setting, using a formula of Hadamard which expresses the variation of a Green function under a variation of the boundary (V. Volterra, *Theory of functionals and of integral and integro-differential equations*, Dover (1959)).

E.11.1 Hadamard

$$\int_V d^4x \partial^\mu X_\mu = \int_\Sigma n^\mu X_\mu \tag{E.331}$$

$$\begin{aligned}&(-\Delta_x + m^2)G_\Sigma(x,y) = \delta^{(4)}(x-y), \quad , G_\Sigma(x(s),y) = 0,\\&(-\Delta_x + m^2)\Phi(x) = 0, \quad , x \in V,\ \Phi(x(s)) = \varphi(s)\end{aligned} \tag{E.332}$$

$$\begin{aligned}\Phi(y) &= \int d^4x \delta^{(4)}(x-y)\Phi(x)\\&= \int d^4x \Phi(x)(-\Delta_x + m^2)G_\Sigma(x,y)\\&= \int d^4x \Phi(x)(-\Delta_x + m^2)G_\Sigma(x,y) - G_\Sigma(x,y)(-\Delta_x + m^2)\Phi(x)\\&= -\int d^4x \left(\Phi(x)\partial^\mu\partial_\mu G_\Sigma(x,y) - G_\Sigma(x,y)\partial^\mu\partial_\mu\Phi(x)\right)\\&= -\int d^4x \partial_\mu \left(\Phi(x)\partial_\mu G_\Sigma(x,y) - G_\Sigma(x,y)\partial_\mu\Phi(x)\right)\\&= -\int d\Sigma(s) n^\mu(\Phi(x)\partial_\mu G_\Sigma(x,y) - 0)\end{aligned} \tag{E.333}$$

$$\Phi(y) = -\int d\Sigma(s) n^\mu \varphi(s) n^\mu(s) \frac{\partial G_\Sigma(x(s),y)}{\partial x^\mu} \tag{E.334}$$

E.12 Local and Global Particles

E.12.1 Quick Reminder: the harmonic Oscillator

The SHO's dynamics is governed by the Hamiltonian

$$H_0 = \frac{1}{2m}(p^2 + m^2\omega^2 q^2). \tag{E.335}$$

The state space of the quantum theory is $\mathcal{H} = L_2[\mathbb{R}, dq]$ formed by the functions $\psi(q)$.

The time-independent Schödinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(q)}{dq^2} + \frac{m}{2}\omega^2 q^2 \psi(q) = E\psi(q). \tag{E.336}$$

We introduce the variable

$$q = \sqrt{\frac{\hbar}{m\omega}}\zeta \tag{E.337}$$

the Schödinger equation is then

$$\frac{\hbar\omega}{2}\left(\frac{d^2}{d\zeta^2} + \zeta^2\right)\psi(\zeta) = E\psi(\zeta). \tag{E.338}$$

If one defines

$$a^\dagger = \frac{1}{\sqrt{2}}\left(-\frac{d}{d\zeta} + \zeta\right). \tag{E.339}$$

as the creation operator and

$$a = \frac{1}{\sqrt{2}}\left(\frac{d}{d\zeta} + \zeta\right). \tag{E.340}$$

as the annihilator operator, the Schödinger equation for a harmonic oscillator reduces to

$$\hbar\omega\left(a^\dagger a + \frac{1}{2}\right)\psi(\zeta) = E\psi(\zeta). \tag{E.341}$$

Note

$$\begin{aligned}
[a, a^\dagger] &= \frac{1}{2}[\left(\frac{d}{d\zeta} + \zeta\right), \left(-\frac{d}{d\zeta} + \zeta\right)] \\
&= \frac{1}{2}([\frac{d}{d\zeta}, \zeta] + [\zeta, -\frac{d}{d\zeta}]) \\
&= 1.
\end{aligned} \tag{E.342}$$

In general

$$|n >= \frac{(a^\dagger)^n}{\sqrt{n!}} \tag{E.343}$$

The solutions of the corresponding time-independent Schödinger equation are

$$\psi_n(q) = < q|n >= \left(\frac{1}{\pi\epsilon^2}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^n n!}} H_n\left(\frac{q}{\epsilon}\right) e^{-q^2/2\epsilon^2} \tag{E.344}$$

where

$$\epsilon = \sqrt{\frac{\hbar}{m\omega}} \tag{E.345}$$

and $H_n(\zeta)$ are the Hermite polynomials, the first few being:

$$\begin{aligned} H_0(\zeta) &= 1 \\ H_1(\zeta) &= 2\zeta \\ H_2(\zeta) &= 4\zeta^2 - 2. \end{aligned} \tag{E.346}$$

the first few wavefunctions being:

$$\begin{aligned} \psi_0(q) &= \left(\frac{1}{\pi\epsilon^2}\right)^{\frac{1}{4}} e^{-q^2/2\epsilon^2} \\ \psi_1(q) &= \left(\frac{1}{\pi\epsilon^2}\right)^{\frac{1}{4}} \sqrt{2}\left(\frac{q}{\epsilon}\right) e^{-q^2/2\epsilon^2} \\ \psi_2(q) &= \left(\frac{1}{\pi\epsilon^2}\right)^{\frac{1}{4}} \left(\frac{1}{2}\right)^{\frac{3}{2}} \left(4\left(\frac{q}{\epsilon}\right)^2 - 2\right) e^{-q^2/2\epsilon^2}. \end{aligned} \tag{E.347}$$

The eigenvalues are

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \qquad n = 0, 1, 2, \ldots \tag{E.348}$$

E.12.2 Two Oscillators

To begin with, we consider two weakly coupled harmonic oscillators q_1, q_2 with unit mass and with the same angular frequency ω; the dynamics is governed by the Hamiltonian

$$H_0 = H_1 + H_2 + V = \frac{1}{2}(p_1^2 + \omega^2 q_1^2) + \frac{1}{2}(p_2^2 + \omega^2 q_2^2) + \lambda q_1 q_2. \tag{E.349}$$

where p_1, p_2 are the momenta conjugate to q_1, q_2 and, say, $\lambda \ll \omega^2$. The state space of the system is $\mathcal{H} = L_2[\mathbb{R}^2, dq_1 dq_2]$ formed by the functions $\psi(q_1, q_2)$. We can define an orthonormal basis in this Hilbert space by diagonalising a complete set of commuting self-adjoint operators. We choose the set formed by the operators H_1 and H_2. Denote E_1 and E_2 the eigenvalues of the operators H_1 and H_2 respectively, and $|n_1, n_2>_{loc}$ their common eigenstates. The reason for the suffix "loc" will be clear in a moment. The integers n_1 and n_2 are the quantum numbers of E_1 and E_2 and we can interpret them as the number of quanta in the first and second oscillator respectively. More precisely, if we measure H_1 of the first oscillator we observe that the result of the measurement outcome is quantised: $E_1 = \hbar\omega(n_1 + 1/2)$ and n_1 can be interpreted as the number of quanta in q_1. It is suggestive to call these quanta "particles". Call $N_{12} = n_1 + n_2$ the total particle number. Introducing a Fock-like notation, we can write the state with no particles also as

$$|0>_{loc} = |0, 0>_{loc}; \tag{E.350}$$

the two one-particle states with particles localised on each oscillator as

$$\begin{aligned} |1>_{loc} &= |1, 0>_{loc}, &\text{(E.351)}\\ |2>_{loc} &= |0, 1>_{loc}, &\text{(E.352)} \end{aligned}$$

where $|1>_{loc}$ represents a particle on the first oscillator and the state $|2>_{loc}$ represents a particle on the second oscillator. Notice that, according to standard Fock-space terminology, any linear combination of one-particle states

$$|\psi>_{loc} = c_1|1>_{loc} + c_2|2>_{loc} \tag{E.353}$$

is also called a one-particle state.

Let us introduce normal coordinates:

$$q_a = \frac{q_1 + q_2}{\sqrt{2}}, \qquad q_b = \frac{q_1 - q_2}{\sqrt{2}} \tag{E.354}$$

We are then able to factorise the hamiltonian as

$$H_0 = H_a + H_b = \frac{1}{2}(p_1^2 + \omega_1^2 q_1^2) + \frac{1}{2}(p_2^2 + \omega_2^2 q_2^2). \tag{E.355}$$

where

$$\omega_1^2 = \omega^2 + \lambda, \qquad \omega_2^2 = \omega^2 - \lambda. \tag{E.356}$$

Let E_a (E_b) be the eigenvalues of H_a (H_b), and denote $|n_a, n_b>$ the common eigenstates of $H_a + H_b$. The number n_a (n_b) is the number of quanta (or "particles") in the mode a (b). Call $N_{ab} = n_a + n_b$ the total number of these particles in the system. For instance the no-particle state is

$$|0 >= |0, 0 >; \tag{E.357}$$

the two one-particle states with particles localised on each mode are

$$\begin{aligned} |a > &= |1, 0 >, \\ |b > &= |0, 1 > . \end{aligned} \tag{E.358}$$

A generic one-particle state is a state of the form

$$|\psi >= c_a|a > +c_b|b > . \tag{E.359}$$

What is the relation between the one-particle states $|\psi >_{loc}$ defined by (E.353) and the one-particle states $|\psi >$ defined in (E.359)?

Denote it

$$|1 >= \frac{1}{\sqrt{2}}|a > + \frac{1}{\sqrt{2}}|b > . \tag{E.360}$$

Is this state equal to $|1 >_{loc}$? No. If λ is small the two states differ slightly, but they do differ. Both states are, in some sense, "one-particle states" and in both states the "particle" is on the first oscillator. However, they are distinct states.

We illustrate the difference in two ways.

Explicit comparison

First, we can simply write both of them explicitly in the coordinate basis.

$$
\begin{aligned}
< q_1, q_2|1 >_{loc} &= < q_1, q_2|1, 0 >_{loc} \\
&= \psi_1(q_1)\psi_0(q_2) \\
&= \left(\frac{1}{\pi\epsilon^2}\right)^{\frac{1}{4}} 2\left(\frac{q_1}{\epsilon}\right)\frac{1}{\sqrt{2}}e^{-q_1^2/2\epsilon^2} \times \left(\frac{1}{\pi\epsilon^2}\right)^{\frac{1}{4}} e^{-q_2^2/2\epsilon^2} \\
&= \sqrt{\frac{2\omega^2}{\pi}} q_1 e^{-\frac{\omega}{2}(q_1^2+q_2^2)} \qquad \text{(E.361)}
\end{aligned}
$$

while

$$
\begin{aligned}
< q_1, q_2|1 > &= \frac{< q_1, q_2|a > + < q_1, q_2|b >}{\sqrt{2}} \\
&= \frac{1}{\sqrt{2}}(< q_1, q_2|1, 0 > + < q_1, q_2|0, 1 >) \\
&= \frac{1}{\sqrt{2}}\psi_1^{(\omega_a)}\left(\frac{q_1+q_2}{\sqrt{2}}\right)\psi_0^{(\omega_b)}\left(\frac{q_1-q_2}{\sqrt{2}}\right) + \frac{1}{\sqrt{2}}\psi_0^{(\omega_a)}\left(\frac{q_1+q_2}{\sqrt{2}}\right)\psi_1^{(\omega_b)}\left(\frac{q_1-q_2}{\sqrt{2}}\right) \\
&= \frac{1}{\sqrt{2}}\cdot\left(\frac{\omega_a}{\pi}\right)^{\frac{1}{4}} 2\left(\sqrt{\omega_a}\cdot\frac{q_1+q_2}{\sqrt{2}}\right)\frac{1}{\sqrt{2}}e^{-\frac{\omega_a}{4}(q_1+q_2)^2} \times \left(\frac{\omega_b}{\pi}\right)^{\frac{1}{4}} e^{-\frac{\omega_b}{4}(q_1-q_2)^2} \\
&\quad + \frac{1}{\sqrt{2}}\cdot\left(\frac{\omega_a}{\pi}\right)^{\frac{1}{4}} e^{-\frac{\omega_a}{4}(q_1+q_2)^2} \times \left(\frac{\omega_b}{\pi}\right)^{\frac{1}{4}} 2\left(\sqrt{\omega_b}\cdot\frac{q_1-q_2}{\sqrt{2}}\right)\frac{1}{\sqrt{2}}e^{-\frac{\omega_b}{4}(q_1-q_2)^2} \\
&= \sqrt{\frac{2}{\pi}}(\omega_a\omega_b)^{\frac{1}{4}}\left(\frac{\sqrt{\omega_a}+\sqrt{\omega_b}}{2}q_1 + \frac{\sqrt{\omega_a}-\sqrt{\omega_b}}{2}q_2\right) e^{-\frac{1}{2}\left(\frac{\omega_a+\omega_b}{2}(q_1^2+q_2^2)+(\omega_a-\omega_b)q_1q_2\right)}
\end{aligned}
$$

(E.362)

If λ is small, $\omega_a \sim \omega_b \sim \omega$ and the two states are similar. In fact, we can compute that their scalar product is

$$
{}_{loc}< 1|1 >= 1 - \mathcal{O}(\lambda^2). \qquad \text{(E.363)}
$$

(See worked exercises).

Comparison via perturbation theory in λ

Second, we can compare them using perturbation theory in λ. This is instructive because we will be able to do the same in the context of field theory. Let us take $H_0 = H_1 + H_2$ as the unperturbed hamiltonian. The two states $|1 >_{loc}$ and $|2 >_{loc}$ span a degenerate eigenspace of H_0.

Recall the theroem regarding simultaneous eigfunctions of operators that commute; if an operator $\hat{Q}$ commutes with V, i.e. $[V, \hat{Q}] = 0$, then they have simultaneous eigenfunctions. The interaction term $\lambda q_1 q_2$ has the "symmetry" under the exchange $q_1 \leftrightarrow q_2$. Let us call the operator $\hat{S}$ where

$$\hat{S}\psi(q_1, q_2) = \psi(q_2, q_1) \tag{E.364}$$

Then

$$\begin{aligned} \hat{S}V(f(q_1, q_2)) &= \hat{S}(Vf(q_1, q_2)) \\ &= \hat{S}(\lambda q_1 q_2 f(q_1, q_2)) \\ &= \lambda q_2 q_1 f(q_2, q_1) \\ &= V\hat{S}f(q_1, q_2) \end{aligned} \tag{E.365}$$

where $f(q_1, q_2)$ is a test function. This implies that $[\hat{S}, V] = 0$. Obviously $\hat{S}^2 = \hat{\mathbb{1}}$, and therefore if $\hat{S}\psi = \beta\psi$, then

$$\begin{aligned} \hat{S}^2\psi(q_1, q_2) &= \beta^2\psi(q_1, q_2) \\ &= \psi(q_1, q_2) \end{aligned} \tag{E.366}$$

and so $\beta = \pm 1$. If $\hat{S}\psi_1(q_1, q_2) = \psi_2(q_1, q_2)$ then

$$\hat{S}\frac{\psi_1(q_1, q_2) \pm \psi_2(q_1, q_2)}{\sqrt{2}} = \pm\frac{(\psi_1(q_1, q_2) \pm \psi_2(q_1, q_2)}{\sqrt{2}}. \tag{E.367}$$

Clearly V is diagonalised in the above degenerate eigensubspace by the two states

$$\begin{aligned} |a>_0 &= \frac{|1>_{loc} + |2>_{loc}}{\sqrt{2}} \\ |b>_0 &= \frac{|1>_{loc} - |2>_{loc}}{\sqrt{2}} \end{aligned} \tag{E.368}$$

We can compute the first order correction to these states using first order perturbation theory. It is convenient to use creation and annihilation operators. From (E.337), (E.339) and (E.340) we have

$$
\begin{aligned}
q_{1,2} &= \frac{1}{\sqrt{2\omega}}(a_{1,2} + a_{1,2}^\dagger), \\
p_{1,2} &= \frac{-i\sqrt{\omega}}{\sqrt{2}}(a_{1,2} - a_{1,2}^\dagger)
\end{aligned}
\tag{E.369}
$$

In terms of the which the perturbation reads

$$
V = \frac{\lambda}{2\omega}(a_1^\dagger a_2^\dagger + a_1 a_2 + a_1^\dagger a_2 + a_1 a_2^\dagger). \tag{E.370}
$$

Notice that the term $a_1^\dagger a_2^\dagger$ takes us out of the one particle sector, giving the non-vanishing matrix elements

$$
\begin{aligned}
{}_{loc}< 2,1|V|a>_0 &= \frac{\lambda}{2\omega}\ {}_{loc}< 2,1|(a_1^\dagger a_2^\dagger + a_1 a_2 + a_1^\dagger a_2 + a_1 a_2^\dagger)(\frac{|1,0>_{loc} + |0,1>_{loc}}{\sqrt{2}}) \\
&= \frac{\lambda}{2\omega}
\end{aligned}
\tag{E.371}
$$

where we have used that

$$
|2,1>_{loc} = \frac{(a_1^\dagger)^2}{\sqrt{2}} a_2^\dagger |0,0>_{loc} = a_1^\dagger a_2^\dagger \frac{1}{\sqrt{2}} |1,0>_{loc}, \tag{E.372}
$$

and similarly

$$
\begin{aligned}
{}_{loc}< 1,2|V|a>_0 &= \frac{\lambda}{2\omega} \\
{}_{loc}< 2,1|V|b>_0 &= \frac{\lambda}{2\omega} \\
{}_{loc}< 1,2|V|b>_0 &= -\frac{\lambda}{2\omega}.
\end{aligned}
\tag{E.373}
$$

To first order in λ, the hamiltonian eigenstates $|a>$ and $|b>$ are therefore

$$
\begin{aligned}
|a> &= |a>_0 + \frac{{}_{loc}< 2,1|V|a>_0}{E_{a_0} - E_{(2,1)_0}} |2,1>_{loc} + \frac{{}_{loc}< 1,2|V|a>_0}{E_{a_0} - E_{(1,2)_0}} |1,2>_{loc} \\
&= |a>_0 - \frac{\lambda}{4\omega^2} |2,1>_{loc} - \frac{\lambda}{4\omega^2} |1,2>_{loc}
\end{aligned}
\tag{E.374}
$$

where we have used $E_{a_0} = (3/2)\omega + (1/2)\omega$ and $E_{(2,1)_0} = E_{(1,2)_0} = (5/2)\omega + (3/2)\omega$. Similarly,

$$
\begin{aligned}
|b> &= |b>_0 + \frac{{}_{loc}<2,1|V|b>_0}{E_{a_0} - E_{(2,1)_0}} \, |2,1>_{loc} + \frac{{}_{loc}<1,2|V|b>_0}{E_{a_0} - E_{(1,2)_0}} \, |1,2>_{loc} \\
&= |b>_0 - \frac{\lambda}{4\omega^2} \, |2,1>_{loc} + \frac{\lambda}{4\omega^2} \, |1,2>_{loc} \, .
\end{aligned}
\tag{E.375}
$$

And therefore, to first order in λ

$$
|1> = |1>_{loc} - \frac{\lambda}{\sqrt{8}\omega^2} \, |2,1>_{loc} \, . \tag{E.376}
$$

Thus, the two states (E.351) and (E.360) are both "one-particle states" in which the particle is concentrated on the oscillator q_1, but they are distinct states. They represent two distinct kinds of one-quantum states, or two distinct kinds of quanta. We call $|1>_{loc}$ a *local* particle state, and $|1>$ a *global* particle state. They represent the simplest example of the distinction between the two classes of states.

More in general, we call "global patricle states" the eigenstates of the "global" number operator

$$
N_{ab}|n_a, n_b> = (n_a + n_b)|n_a, n_b>, \tag{E.377}
$$

and we call "local particle states" the eigenstates of the "local" number operator

$$
N_1|n_1, n_2>_{loc} = n_1|n_1, n_2>_{loc} \, . \tag{E.378}
$$

Let us illustrate the different properties that these states have. The state $|1>_{loc}$ is an eigenstate of H_1, which is an observable that depends just on q_1 and its momentum, namely just on the variable associated to the first oscillator. If we want to measure how many local particles are in the first oscillator, namely to measure n_1, we can make a measurement that involves solely variables of the q_1 oscillator. In this sense $|1>_{loc}$ is "local".

The state $|1>$, on the other hand, describes a single particle "on the first oscillator", but is not an eigenstate of observables that depend on variables of the sole first oscillator. This can be seen from the fact that it is a state in which the two oscillators are (weakly) correlated. The source of these correlations can be traced to the vacuum state: local particles are excitation over the local vacuum (E.350) which has no correlations:

$$< q_1, q_2|0 >_{loc} = \sqrt{\frac{\omega}{\pi}} e^{-\frac{\omega}{2}q_1^2} e^{-\frac{\omega}{2}q_2^2} = \psi_0(q_1)\psi_0(q_2) \tag{E.379}$$

while global particles are excitations over the global vacuum (E.357)

$$< q_1, q_2|0 > = \frac{(\omega_a\omega_b)^{1/4}}{\sqrt{\pi}} e^{-\frac{1}{2}\frac{\omega_a+\omega_b}{2}q_1^2} e^{-\frac{1}{2}\frac{\omega_a+\omega_b}{2}q_2^2} e^{-\frac{1}{2}(\omega_a-\omega_b)q_1q_2} = \psi_0^{(\omega_a)}\left(\frac{q_1+q_2}{\sqrt{2}}\right)\psi_0^{(\omega_b)}\left(\frac{q_1-q_2}{\sqrt{2}}\right) \tag{E.380}$$

which does not factorise (i.e. cannot be put in the form $\psi(q_1)\phi(q_2)$), and therefore represents vacuum correlations between the two oscillators.

What is the physical relevance of the state $|1>$?

Notice that $|1>_{loc}$ is not an energy eigenstate, because of the interaction term V, but $|1>$ isn't an energy eigenstate either, because $|1,0>$ and $|0,1>$ have different energies:

$$\begin{aligned} H|1> &= H\left(\frac{1}{\sqrt{2}}|1,0> + \frac{1}{\sqrt{2}}|0,1>\right) \\ &= (H_a + H_b)\left(\frac{1}{\sqrt{2}}|1,0> + \frac{1}{\sqrt{2}}|0,1>\right) \\ &= 2\omega_a\frac{1}{\sqrt{2}}|1,0> + 2\omega_b\frac{1}{\sqrt{2}}|0,1> \\ &\not\propto |1> . \end{aligned} \tag{E.381}$$

Its defining property is just the fact of being a linear combination of one-quantum excitations of the normal modes of the system. What then is the physical relevance of the state $|1>$? It is the following: the one-particle Fock states of QFT are precisely states of the same kind as $|1>$. To see this, consider the following: one-particle Fock states of QFT are precisely states of the same kind as $|1>$. To see this, consider a Fock particle localised in a region R. This state can be described by means of a function $f(x)$ with compact support in R, as

$$|f> = \int dk\tilde{f}(k)|k> \tag{E.382}$$

where $\tilde{f}(k)$ is the Fourier transform of $f(x)$ and the states $|k>$ are the one-particle Fock states with momentum k. They are energy eigenstates (with different energies) and they are single-particle excitations of the normal modes of the system. Therefore they are the analog of the states $|1,0>$ and $|0,1>$of the two-oscillator model. The linear combination (E.382) is the analog of the linear combination (E.360), which picks the one-particle global state maximally concentrated in the region chosen (the oscillator q_1 in the model, the region R in the QFT). Thus, Fock particles are global particles. No measurement in a finite region R can count these particles, because Fock particles are not eigenstates of local field operators, precisely in the same sense in which $|1>$ is not an eigenstate of an observable localised on the q_1 oscillator. If we make a measurement with an apparatus located in a region R, we can count the number of particles the apparatus detect. However, these particles are not global particles. They are local particles, that can be described by appropriate QFT states which are close, but not identical, to $n-$ particle Fock states, like $|1>_{loc}$ is close, but not identical to $|1>$. Later on we will discuss local particle states, analogous to the $|n_1, n_2>_{loc}$ states, in the context of QFT.

Probability of detector measuring the first oscillator measuring a particle on the first oscillator

Suppose now the state of the system is $|0>$ and we measure whether a particle is on the first oscillator by measuring the energy E_1. The probability of not seeing any particle is not determined by the sole scalar product (E.363), because we are in fact tracing over n_2. Rather it is given by

$$\mathcal{P} = \left| \sum_{n_2} {}_{loc}< 0, n_2 | 0 > \right|^2 = < 0 | P_{0loc} | 0 > \tag{E.383}$$

where

$$P_{0loc} = \sum_{n_2} |0, n_2>_{loc} \ {}_{loc}< 0, n_2| \tag{E.384}$$

is the projection on the lowest eigenspace of H_1.

$$\begin{aligned}
\mathcal{P} &= \left| \sum_{n_2} \int dq_1 dq_2 \ {}_{loc}< 0, n_2 | q_1, q_2 >< q_1, q_2 | 0 > \right|^2 \\
&= \left| \sum_{n_2} \int dq_1 dq_2 \psi_0^{(\omega)*}(q_1) \psi_{n_2}^{(\omega)*}(q_2) \ \psi_0^{(\omega_a)} \left(\frac{q_1 + q_2}{\sqrt{2}} \right) \psi_0^{(\omega_b)} \left(\frac{q_1 - q_2}{\sqrt{2}} \right) \right|^2
\end{aligned} \tag{E.385}$$

E.12.3 Chain of Oscillators

As an intermediate step before moving on to field theory, we consider a chain of harmonic oscillators. This system allows one to emphasise several important points regarding the relation between local and global particle states.

We study a system of n harmonic oscillators $\mathbf{q} = (q_i)$, $i = 1, \ldots, n$ with the same frequencies $\omega = 1$ and coupled by a constant λ. Each oscillator is coupled with its two neighbouring (except for the first and last oscillator that have only one coupling)

$$H = \frac{1}{2}\left(|\mathbf{p}|^2 + |\mathbf{q}|^2\right) + \lambda \sum_{i=1}^{n-1} q^i q^{i+1} \tag{E.386}$$

where $|\mathbf{q}|^2 = \sum_i (q^i)^2$. Notice that we are not considering a ring but an open chain of oscillators. Diagonalising the hamiltonian of the system we obtain the normal frequencies

$$\omega_a = \sqrt{1 + 2\lambda \cos\theta_a}, \qquad \text{where} \quad \theta_a = \frac{a\pi}{n+1}, \qquad \text{and} \quad a = 1, \ldots, n. \tag{E.387}$$

The normal modes $\mathbf{Q} = (Q_a)$, $a = 1, \ldots, n$ are given by $\mathbf{Q} = U^{(n)}\mathbf{q}$, where $U^{(n)}$ is the orthogonal $n \times n$ matrix

$$U^{(n)}_{ai} = \sqrt{\frac{2}{n+1}} \sin\left(\frac{ai\pi}{n+1}\right). \tag{E.388}$$

The vacuum state is

$$< \mathbf{q}|0 >= \prod_{a=1}^{n} \left(\frac{\omega_a}{\pi}\right)^{1/4} e^{-\frac{1}{2} q^i D^{(n)}_{ij} q^j}, \tag{E.389}$$

where

$$D^{(n)}_{ij} = \sum_a U^{(n)}_{ai} \omega_a U^{(n)}_{aj}. \tag{E.390}$$

(See worked exercises).

A basis that diagonalises H is given by the states $|\mathbf{n} >= |n_1, \ldots, n_n >$ with n_a quanta in the $a-$th mode. The number operator is

$$N|\mathbf{n}>= \left(\sum_{a=1}^{n} n_a\right)|\mathbf{n}> . \tag{E.391}$$

Denote $|a>$ the one particle state $|0,\ldots,1,\ldots,0>$ in which the vacuum state except for the $a-$th mode which is in its first excitation. The state

$$|i>= \sum_{a=1}^{n} U^{-1}_{ia}|a> \tag{E.392}$$

is the one particle state maximally concentrated on the $i-$th oscillator. It is the analog of the global one particale states (E.360) and (). This is the global one-particle state, with the particle on the $i-$th oscillator.

Partitioning the chain

Now, consider a partition of the chain in two regions R_1 and R_2. Let the region R_1 be formed by the first n_1 oscillators, and the region R_2 be formed by the remaining n_2 oscillators, with $n_1+n_2=n$. We write $\mathbf{q}=(\mathbf{q}_1,\mathbf{q}_2)$, where $\mathbf{q}_1$ (respectively $\mathbf{q}_2$) is a vector with n_1 (n_2) components. We regard the first region of oscillators as a generalisation of the oscillator q_1 in the previous section, and the second region as the analog of the oscillator q_2 . The total Hilbert space of the system factorises as $\mathcal{H}=\mathcal{H}_1\otimes\mathcal{H}_2$. We can rewrite the hamiltonian (E.386) in the form

$$\begin{aligned} H &= H_1 + H_2 + V \\ &= \left(\frac{1}{2}\left(|\mathbf{p}_1|^2+|\mathbf{q}_1|^2\right)+\lambda\sum_{i=1}^{n_1-1} q_1^i q_1^{i+1}\right)+\left(\frac{1}{2}\left(|\mathbf{p}_2|^2+|\mathbf{q}_2|^2\right)+\lambda\sum_{i=1}^{n_2-1} q_2^i q_2^{i+1}\right)+\lambda q_1^{n_1} q_2^1. \end{aligned} \tag{E.393}$$

E.12.4 Convergence Between Local and Global States

E.13 Worked Exercises and Details

Hamilton Function

Proposition: Hamilton function for a harmonic oscillator

Prove that the Hamilton function of a harmonic oscillator is

$$S(q,t,q',t') = m\omega\frac{(q^2+{q'}^2)cos\omega(t-t') - 2qq'}{2\sin\omega(t'-t)}$$

for motion that starts at (q,t) and ends at (q',t').

Solution

First we need the solution of

$$\ddot{q} = -\frac{k}{m}q(\tilde{t}) = -\omega^2 q(\tilde{t})$$

with boundary conditions $q = q(\tilde{t} = t)$ and $q' = q(\tilde{t} = t')$. It is well know the general solution is of the form $A\cos(\omega\tilde{t}) + B\sin(\omega\tilde{t})$. The solution with correct boundary conditions is easily seen to be

$$q_{qtq't'}(\tilde{t}) = \frac{q\sin(\omega t') - q'\sin(\omega t)}{\sin\omega(t'-t)}\cos(\omega\tilde{t}) + \frac{q'\cos(\omega t) - q\cos(\omega t')}{\sin\omega(t'-t)}\sin(\omega\tilde{t}) \tag{E.394}$$

This simplifies

$$\begin{aligned} q_{qtq't'}(\tilde{t}) &= \frac{q[\sin(\omega t')\cos(\omega\tilde{t}) - \cos(\omega t')\sin(\omega\tilde{t})] + q'[\sin(\omega\tilde{t})\cos(\omega t) - \cos(\omega\tilde{t})\sin(\omega t)]}{\sin\omega(t'-t)} \\ &= \frac{q\sin\omega(t'-\tilde{t}) + q'\sin\omega(\tilde{t}-t)}{\sin\omega(t'-t)}. \end{aligned} \tag{E.395}$$

The velocity is then

$$\dot{q}_{qtq't'}(\tilde{t}) = \frac{-q\cos\omega(t'-\tilde{t}) + q'\cos\omega(\tilde{t}-t)}{\sin\omega(t'-t)}. \tag{E.396}$$

The Hamilton function is

$$
\begin{aligned}
S(q,t,q',t') &= \int_t^{t'} d\tilde{t}\left(\frac{1}{2}m\dot{q}^2_{qtq't'} - \frac{1}{2}kq^2_{qtq't'}\right) \\
&= \frac{m\omega^2}{2\sin^2\omega(t'-t)}\int_t^{t'} d\tilde{t}\,\big[\{-q\cos\omega(t'-\tilde{t}) + q'\cos\omega(\tilde{t}-t)\}^2 \\
&\qquad -\{q\sin\omega(t'-\tilde{t}) + q'\sin\omega(\tilde{t}-t)\}^2\big] \\
&= \frac{m\omega^2}{2\sin^2\omega(t'-t)}\int_t^{t'} d\tilde{t}\Big[q^2(\cos^2\omega(t'-\tilde{t}) - \sin^2\omega(t'-\tilde{t})) \\
&\qquad +{q'}^2(\cos^2\omega(\tilde{t}-t) - \sin^2\omega(\tilde{t}-t)) \\
&\qquad -2qq'\big(\cos\omega(t'-\tilde{t})\cos\omega(\tilde{t}-t) + \sin\omega(t'-\tilde{t})\sin\omega(\tilde{t}-t)\big)\Big] \\
&= \frac{m\omega^2}{2\sin^2\omega(t'-t)}\int_t^{t'} d\tilde{t}\Big[q^2\cos 2\omega(t'-\tilde{t}) + {q'}^2\cos 2\omega(\tilde{t}-t) - 2qq'\cos\omega(2\tilde{t}-t-t')\Big] \\
&= \frac{m\omega^2}{2\sin^2\omega(t'-t)}\Big(q^2\frac{1}{2\omega}\Big[-\sin 2\omega(t'-\tilde{t})\Big]_t^{t'} + {q'}^2\frac{1}{2\omega}\Big[\sin 2\omega(\tilde{t}-t)\Big]_t^{t'} \\
&\quad -2qq'\frac{1}{2\omega}\Big[\sin\omega(2\tilde{t}-t-t')\Big]_t^{t'}\Big) \\
&= \frac{m\omega^2}{2\sin^2\omega(t'-t)}\left((q^2+{q'}^2)\frac{1}{2\omega}\sin 2\omega(t'-t) - 2qq'\frac{1}{2\omega}(2\sin\omega(t'-t))\right) \\
&= \frac{m\omega^2}{2\sin^2\omega(t'-t)}\left((q^2+{q'}^2)\frac{1}{2\omega}2\sin\omega(t-t')\cos\omega(t-t') - 2qq'\frac{1}{2\omega}(2\sin\omega(t'-t))\right) \\
&= m\omega\frac{(q^2+{q'}^2)cos\omega(t-t') - 2qq'}{2\sin\omega(t'-t)}. \qquad \text{(E.397)}
\end{aligned}
$$

Expansion in λ.

Idenity: Expansion in λ.

Prove that

$$
e^{-\lambda(T+V)/N} = e^{-\lambda T/N}e^{-\lambda V/N} + \mathcal{O}\left(\frac{\lambda^2}{N^2}\right) \qquad \text{(E.398)}
$$

where T and V are operators and that the coefficent of λ^2/N^2 is given by the commutator $\frac{1}{2}[V,T]$.

Solution

We define the operator-valued function of the parameter λ

$$F(\lambda) := e^{\lambda T/N} e^{-\lambda(T+V)/N} e^{\lambda V/N} \tag{E.399}$$

It can be expanded as a Taylor series about $\lambda = 0$

$$F(\lambda) := \mathbb{1} + \sum_{n=1}^{\infty} \frac{1}{n!} \left(\frac{d^n F}{d\lambda^n} \right)_{\lambda=0} \lambda^n \tag{E.400}$$

where we have used $F(0) = \mathbb{1}$. Taking the first derivative gives

$$\begin{aligned}
\frac{d}{d\lambda} F(\lambda) &= \frac{d}{d\lambda} \left\{ e^{\lambda T/N} e^{-\lambda(T+V)/N} e^{\lambda V/N} \right\} \\
&= \frac{1}{N} \Big(e^{\lambda T/N} T e^{-\lambda(T+V)/N} e^{\lambda V/N} - e^{\lambda T/N} (T+V) e^{-\lambda(T+V)/N} e^{\lambda V/N} \\
&\quad + e^{\lambda T/N} e^{-\lambda(T+V)/N} V e^{\lambda V/N} \Big) \\
&= \frac{1}{N} e^{\lambda T/N} [e^{-\lambda(T+V)/N}, V] e^{\lambda V/N}
\end{aligned} \tag{E.401}$$

Putting $\lambda = 0$ we have:

$$\frac{d}{d\lambda} F(\lambda) \Big|_{\lambda=0} = 0 \tag{E.402}$$

as $[\mathbb{1}, V] = 0$. Now consider the second derivative of $F(\lambda)$:

$$\begin{aligned}
\frac{d^2}{d\lambda^2} F(\lambda) &= \frac{1}{N} \frac{d}{d\lambda} \left\{ e^{\lambda T/N} [e^{-\lambda(T+V)/N}, V] e^{\lambda V/N} \right\} \\
&= \frac{1}{N^2} (e^{\lambda T/N} T [e^{-\lambda(T+V)/N}, V] e^{\lambda V/N} \\
&\quad + e^{\lambda T/N} [e^{-\lambda(T+V)/N}, V] V e^{\lambda V/N} \\
&\quad + e^{\lambda T/N} [-e^{-\lambda(T+V)/N} (T+V) V + V (T+V) e^{-\lambda(T+V)/N}] e^{\lambda V/N}).
\end{aligned} \tag{E.403}$$

Putting $\lambda = 0$ and dividing by 2! gives the coefficient of the third term in the Taylor expansion,

$$\frac{1}{2!} \frac{d^2}{d\lambda^2} F(\lambda) \Big|_{\lambda=0} = \frac{1}{N^2} \frac{1}{2} [V, T]. \tag{E.404}$$

Therefore we have:

$$e^{\lambda T/N} e^{-\lambda(T+V)/N} e^{\lambda V/N} = \mathbb{1} + \frac{\lambda^2}{N^2} \frac{1}{2} [V, T] + \mathcal{O} \left(\frac{\lambda^3}{N^3} \right). \tag{E.405}$$

Multiplying by the left with $e^{-\lambda T/N}$ and by the right by $e^{-\lambda V/N}$ gives:

$$\begin{aligned}
e^{-\lambda(T+V)/N} &= e^{-\lambda T/N}e^{-\lambda V/N} + \frac{\lambda^2}{N^2}e^{-\lambda T/N}\left(\frac{1}{2}[V,T]\right)e^{-\lambda V/N} + \mathcal{O}\left(\frac{\lambda^3}{N^3}\right) \\
&= e^{-\lambda T/N}e^{-\lambda V/N} + \frac{\lambda^2}{N^2}\left(\mathbb{1} - \frac{\lambda T}{N} + \dots\right)\frac{1}{2}[V,T]\left(\mathbb{1} - \frac{\lambda V}{N} + \dots\right) + \mathcal{O}\left(\frac{\lambda^3}{N^3}\right) \\
&= e^{-\lambda T/N}e^{-\lambda V/N} + \frac{\lambda^2}{N^2}\frac{1}{2}[V,T] + \mathcal{O}\left(\frac{\lambda^3}{N^3}\right) \qquad \text{(E.406)}
\end{aligned}$$

which is the desired result.

Spacetime Smeared States

Proposition: Spacetime Smeared States

Functional Integral

Proposition: Functional Integral

$$S_T^E[\phi] = \frac{1}{2}\int_0^T dt \int d^3x \left[(\partial_\mu \phi_{\varphi,\Sigma})^2 + m^2\phi_{\varphi,\Sigma}^2\right] \qquad \text{(E.407)}$$

The gausian integral

$$W[\varphi_1, \varphi_2, T] = \int_{\phi|_{t=0}=\varphi_2}^{\phi|_{t=T}=\varphi_1} \mathcal{D}\phi \; e^{S_T^E[\phi]} \qquad \text{(E.408)}$$

can be solved by finding the extremal value of the exponent, that is, by solving the classical equation with boundary conditions

(a) Find the classical solution corresponding to Eq.(E.407).

(b) Do the integral to Eq.(E.408).

$$W[\varphi_1, \varphi_2, T] = \mathcal{N}\exp\left\{-\frac{1}{2}\int \frac{d^3k}{(2\pi)^3}\omega\left(\frac{|\tilde{\varphi}_1|^2 + |\tilde{\varphi}_2|^2}{\tanh(\omega T)} - \frac{2\tilde{\varphi}_1\overline{\tilde{\varphi}_2}}{\sinh(\omega T)}\right)\right\} \qquad \text{(E.409)}$$

where $\omega = \sqrt{k^2 + m^2}$

$$\tilde{\varphi}(k) = \int d^3x e^{ikx} \varphi(x) \tag{E.410}$$

Solutions

(a)

$$\left.\frac{\delta S^E}{\delta \overline{\phi}}\right|_{\overline{\phi}=\phi_{cl}} = 0 \tag{E.411}$$

$$\begin{aligned}
\frac{\delta S^E}{\delta \overline{\phi}} &= \frac{1}{2}\frac{\delta}{\delta \overline{\phi}} \int_0^T dt \left(\int d^3x \left[(\partial_t \phi)^2 - (\partial_i \phi)^2 + m^2 \phi^2 \right] \right) \\
&= \int d^3x \left[-\partial_t^2 \phi + \partial_i^2 \phi + m\phi \right] = 0
\end{aligned} \tag{E.412}$$

$$\begin{aligned}
\phi_{cl}(x,t) &= \int \frac{d^3k d^3y}{(2\pi)^3} e^{-i\vec{k}(\vec{x}-\vec{y})} \; \frac{\varphi_2(\vec{y}) \sinh(\omega t) - \varphi_1(\vec{y}) \sinh(\omega(t-T))}{\sinh(\omega T)} \\
&= \int \frac{d^3k}{(2\pi)^3} e^{-i\vec{k}\vec{x}} \; \frac{\tilde{\varphi}_2(\vec{k}) \sinh(\omega t) - \tilde{\varphi}_1(\vec{k}) \sinh(\omega(t-T))}{\sinh(\omega T)}
\end{aligned} \tag{E.413}$$

$$\tilde{\phi}_{cl}(k,t) = \frac{\tilde{\varphi}_2(\vec{k}) \sinh(\omega t) - \tilde{\varphi}_1(\vec{k}) \sinh(\omega(t-T))}{\sinh(\omega T)} \tag{E.414}$$

(b)

$$S^E[\phi, T] = S^E[\overline{\phi}, T] + \left.\frac{\delta S^E}{\delta \overline{\phi}}\right|_{\overline{\phi}=\phi_{cl}} (\overline{\phi} - \phi_{cl}) + \left.\frac{\delta^2 S^E}{\delta \phi^2}\right|_{\overline{\phi}=\phi_{cl}} (\overline{\phi} - \phi_{cl})^2 \tag{E.415}$$

Taylor expansion

$$\phi_{cl} = \varphi_2 \frac{\sinh(\omega(T-t))}{\sinh(\omega T)} + \varphi_1 \frac{\sinh(\omega t)}{\sinh(\omega T)} \tag{E.416}$$

so that the first term in the Taylor expansion is

$$S^E[\phi_{cl}] = \frac{1}{2} \frac{\omega}{\sinh(\omega T)} ((\varphi_2^2 + \varphi_1^2) \cosh(\omega T) - 2\varphi_1 \varphi_2) \tag{E.417}$$

$$W[\varphi_1,\varphi_2,T] = \mathcal{N}\exp\left(-\frac{1}{2}\frac{\omega}{\sinh(\omega T)}((\varphi_2^2+\varphi_1^2)\cosh(\omega T) - 2\varphi_1\varphi_2)\right) \tag{E.418}$$

where

$$\mathcal{N} = \int \mathcal{D}\overline{\phi}\exp() \tag{E.419}$$

Lorentzian case

Elementary geometry of an equilateral tetrahedron

Elementary geometry of an equilateral tetrahedron

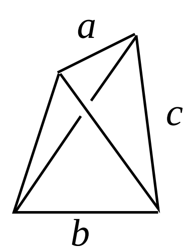

Figure E.4: equiltetra.

$$\sin\frac{\theta_a}{2} = \frac{b}{\sqrt{4c^2-a^2}}, \qquad \sin\frac{\theta_b}{2} = \frac{a}{\sqrt{4c^2-b^2}}, \qquad \sin\frac{\theta_c}{2} = \frac{ab}{\sqrt{(4c^2-a^2)(4c^2-b^2)}} \tag{E.420}$$

Factorising chain of two oscillators

Show that

$$H_0 = \frac{1}{2}(p_1^2+\omega^2 q_1^2) + \frac{1}{2}(p_2^2+\omega^2 q_2^2) + \lambda q_1 q_2 \tag{E.421}$$

factorises to

$$H_0 = \frac{1}{2}(p_a^2 + \omega_a^2 q_a^2) + \frac{1}{2}(p_b^2 + \omega_b^2 q_b^2) \tag{E.422}$$

via the normal coordinates

$$q_a = \frac{q_1 + q_2}{\sqrt{2}}, \qquad q_b = \frac{q_1 - q_2}{\sqrt{2}}. \tag{E.423}$$

Proof:

First

$$\begin{aligned}
\frac{1}{2}(\omega_a^2 q_a^2 + \omega_b^2 q_b^2) &= \frac{1}{2}\left\{\omega_a^2 \left(\frac{q_1 + q_2}{\sqrt{2}}\right)^2 + \omega_b^2 \left(\frac{q_1 - q_2}{\sqrt{2}}\right)^2\right\} \\
&= \frac{1}{2}\left\{\frac{\omega_a^2 + \omega_b^2}{2}(q_1^2 + q_2^2) + (\omega_a^2 - \omega_b^2) q_1 q_2\right\} \\
&\equiv \frac{1}{2}\omega^2 (q_1^2 + q_2^2) + \lambda q_1 q_2
\end{aligned} \tag{E.424}$$

Implying

$$\omega^2 = \frac{\omega_a^2 + \omega_b^2}{2}, \qquad \lambda = \frac{1}{2}(\omega_a^2 - \omega_b^2) \tag{E.425}$$

We find

$$\omega_a^2 = \omega^2 + \lambda, \qquad \omega_b^2 = \omega^2 - \lambda. \tag{E.426}$$

Now we turn to the momenta operators

$$\begin{aligned}
p_1 &= -i\hbar \frac{\partial}{\partial q_1} \\
&= -i\hbar \left(\frac{\partial q_a}{\partial q_1}\frac{\partial}{\partial q_a} + \frac{\partial q_b}{\partial q_1}\frac{\partial}{\partial q_b}\right) \\
&= -i\hbar \frac{1}{\sqrt{2}}\left(\frac{\partial}{\partial q_a} + \frac{\partial}{\partial q_b}\right)
\end{aligned} \tag{E.427}$$

similarly

$$p_2 = -i\hbar \frac{1}{\sqrt{2}}\left(\frac{\partial}{\partial q_a} - \frac{\partial}{\partial q_b}\right). \tag{E.428}$$

Then

$$
\begin{aligned}
p_1^2 + p_2^2 &= -\hbar^2 \frac{1}{2} \left\{ \left(\frac{\partial}{\partial q_a} + \frac{\partial}{\partial q_b} \right)^2 + \left(\frac{\partial}{\partial q_a} - \frac{\partial}{\partial q_b} \right)^2 \right\} \\
&= -\hbar^2 \frac{\partial^2}{\partial q_a^2} + -\hbar^2 \frac{\partial^2}{\partial q_b^2} \\
&= p_1^2 + p_2^2.
\end{aligned}
\tag{E.429}
$$

$\boxed{}$

$\boxed{\text{Comparison of local and global states for two oscillators.}}$

Take

$$
\omega_a^2 = \omega^2 + \lambda, \qquad \omega_b^2 = \omega^2 - \lambda \tag{E.430}
$$

and attempt an expansion of

$$
< q_1, q_2 | 0 >= \sqrt{\frac{2}{\pi}} (\omega_a \omega_b)^{\frac{1}{4}} \left(\frac{\sqrt{\omega_a} + \sqrt{\omega_b}}{2} q_1 + \frac{\sqrt{\omega_a} - \sqrt{\omega_b}}{2} q_2 \right) e^{-\frac{1}{2}\left(\frac{\omega_a + \omega_b}{2} (q_1^2 + q_2^2) + (\omega_a - \omega_b) q_1 q_2 \right)} \tag{E.431}
$$

in λ. How does it compare to

$$
\sqrt{\frac{2\omega^2}{\pi}} q_1 e^{-\frac{\omega}{2}(q_1^2 + q_2^2)} ?. \tag{E.432}
$$

Proof:

Note:

$$
\begin{aligned}
(\omega_a \omega_b)^{\frac{1}{4}} &= (\omega^4 - \lambda^2)^{\frac{1}{8}} \\
&= \sqrt{\omega} \left(1 - \frac{1}{8} \frac{\lambda^2}{\omega^4} + \mathcal{O}(\lambda^4) \right)
\end{aligned}
\tag{E.433}
$$

$$
\begin{aligned}
\frac{\sqrt{\omega_a}+\sqrt{\omega_b}}{2} &= \frac{1}{2}\left(\omega^2+\lambda\right)^{\frac{1}{4}}+\frac{1}{2}\left(\omega^2-\lambda\right)^{\frac{1}{4}} \\
&= \frac{\sqrt{\omega}}{2}\left(1+\frac{1}{4}\frac{\lambda}{\omega^2}-\frac{3}{4^2}\frac{1}{2!}\frac{\lambda^2}{\omega^4}+\mathcal{O}(\lambda^3)\right)+\frac{\sqrt{\omega}}{2}\left(1-\frac{1}{4}\frac{\lambda}{\omega^2}-\frac{3}{4^2}\frac{1}{2!}\frac{\lambda^2}{\omega^4}+\mathcal{O}(\lambda^3)\right) \\
&= \sqrt{\omega}\left(1-\frac{3}{4^2}\frac{1}{2!}\frac{\lambda^2}{\omega^4}+\mathcal{O}(\lambda^4)\right) \\
&= \sqrt{\omega}\left(1-\frac{3}{32}\frac{\lambda^2}{\omega^4}+\mathcal{O}(\lambda^4)\right) \qquad \text{(E.434)}
\end{aligned}
$$

$$
\frac{\sqrt{\omega_a}-\sqrt{\omega_b}}{2} = \sqrt{\omega}\left(\frac{1}{4}\frac{\lambda}{\omega^2}+\mathcal{O}(\lambda^3)\right) \qquad \text{(E.435)}
$$

$$
\begin{aligned}
\frac{\omega_a+\omega_b}{2} &= \frac{1}{2}(\omega^2+\lambda)^{\frac{1}{2}}+\frac{1}{2}(\omega^2-\lambda)^{\frac{1}{2}} \\
&= \frac{\omega}{2}\left(1+\frac{1}{2}\frac{\lambda}{\omega^2}-\frac{1}{2^2}\frac{1}{2!}\frac{\lambda^2}{\omega^4}+\mathcal{O}(\lambda^3)\right)+\frac{\omega}{2}\left(1-\frac{1}{2}\frac{\lambda}{\omega^2}-\frac{1}{2^2}\frac{1}{2!}\frac{\lambda^2}{\omega^4}+\mathcal{O}(\lambda^3)\right) \\
&= \omega\left(1-\frac{1}{2^2}\frac{1}{2!}\frac{\lambda^2}{\omega^4}+\mathcal{O}(\lambda^4)\right) \\
&= \omega\left(1-\frac{1}{8}\frac{\lambda^2}{\omega^4}+\mathcal{O}(\lambda^4)\right) \qquad \text{(E.436)}
\end{aligned}
$$

$$
\begin{aligned}
\omega_a-\omega_b &= (\omega^2+\lambda)^{\frac{1}{2}}-(\omega^2-\lambda)^{\frac{1}{2}} \\
&= \omega\left(1+\frac{1}{2}\frac{\lambda}{\omega^2}-\frac{1}{2^2}\frac{1}{2!}\frac{\lambda^2}{\omega^4}+\mathcal{O}(\lambda^3)\right)-\omega\left(1-\frac{1}{2}\frac{\lambda}{\omega^2}-\frac{1}{2^2}\frac{1}{2!}\frac{\lambda^2}{\omega^4}+\mathcal{O}(\lambda^3)\right) \\
&= \omega\left(\frac{1}{2}\frac{\lambda}{\omega^2}+\mathcal{O}(\lambda^3)\right) \qquad \text{(E.437)}
\end{aligned}
$$

Inserting these into (E.431) we see

$$
\begin{aligned}
< q_1, q_2|0 > &= \sqrt{\frac{2}{\pi}}\times\sqrt{\omega}\left(1-\frac{1}{8}\frac{\lambda^2}{\omega^4}+\mathcal{O}(\lambda^4)\right)\times\left\{\sqrt{\omega}\left(1-\frac{3}{4^2}\frac{1}{2!}\frac{\lambda^2}{\omega^4}+\mathcal{O}(\lambda^3)\right)q_1+\right. \\
&\left.\sqrt{\omega}\left(\frac{1}{4}\frac{\lambda}{\omega^2}+\mathcal{O}(\lambda^3)\right)q_2\right\}\times\exp\left\{-\frac{1}{2}\omega\left(1-\frac{1}{2^2}\frac{1}{2!}\frac{\lambda^2}{\omega^4}+\mathcal{O}(\lambda^3)\right)(q_1^2+q_2^2)\right\} \\
&\times\exp\left\{-\frac{1}{2}\omega\left(\frac{1}{2}\frac{\lambda}{\omega^2}+\mathcal{O}(\lambda^3)\right)q_1q_2\right\}
\end{aligned}
\qquad \text{(E.438)}
$$

and with further simplification

$$
\begin{aligned}
< q_1, q_2|0 > \;&=\; \sqrt{\frac{2\omega^2}{\pi}} \left\{ \left(1 - \frac{3}{32}\frac{\lambda^2}{\omega^4} + \mathcal{O}(\lambda^3)\right) q_1 + \left(\frac{1}{4}\frac{\lambda}{\omega^2} + \mathcal{O}(\lambda^3)\right) q_2 \right\} \\
&\times\; \exp\left\{ -\frac{1}{2}\omega \left(1 - \frac{1}{8}\frac{\lambda^2}{\omega^4} + \mathcal{O}(\lambda^3)\right)(q_1^2 + q_2^2) \right\} \exp\left\{ -\frac{1}{2}\omega \left(\frac{1}{2}\frac{\lambda}{\omega^2} + \mathcal{O}(\lambda^3)\right) q_1 q_2 \right\}
\end{aligned}
\tag{E.439}
$$

Comparison of local and global states for two oscillators: scalar product.

Calculate the scalar product

$$
{}_{loc} < 0|0 > \tag{E.440}
$$

as an expansion in λ.

Proof:

$$
\begin{aligned}
{}_{loc} < 1|1 > \;&=\; \int dq_1 dq_2 \; {}_{loc} < 1|q_1, q_2 >< q_1, q_2|1 > \\
&=\; \int dq_1 dq_2 \sqrt{\frac{2\omega^2}{\pi}} q_1 e^{-\frac{\omega}{2}(q_1^2+q_2^2)} \times \\
&\times\; \sqrt{\frac{2}{\pi}} (\omega_a \omega_b)^{\frac{1}{4}} \left(\frac{\sqrt{\omega_a} + \sqrt{\omega_b}}{2} q_1 + \frac{\sqrt{\omega_a} - \sqrt{\omega_b}}{2} q_2 \right) e^{-\frac{1}{2}\left(\frac{\omega_a+\omega_b}{2}(q_1^2+q_2^2) + (\omega_a-\omega_b) q_1 q_2\right)} \\
&=\; \frac{2}{\pi}\omega (\omega_a \omega_b)^{\frac{1}{4}} \int dq_1 dq_2 \left(\frac{\sqrt{\omega_a} + \sqrt{\omega_b}}{2} q_1^2 + \frac{\sqrt{\omega_a} - \sqrt{\omega_b}}{2} q_1 q_2 \right) \\
&\quad \times e^{-\frac{1}{2}\left(\frac{\omega_a+\omega_b+2\omega}{2}(q_1^2+q_2^2) + (\omega_a-\omega_b) q_1 q_2\right)}.
\end{aligned}
\tag{E.441}
$$

We need to evaluate integrals of the form:

$$
I_1 = \int dq_1 dq_2 \; q_1^2 e^{-\frac{1}{2}\left(\alpha(q_1^2+q_2^2) + 2\beta q_1 q_2\right)} \tag{E.442}
$$

and

$$
I_2 = \int dq_1 dq_2 \; q_1 q_2 e^{-\frac{1}{2}\left(\alpha(q_1^2+q_2^2) + 2\beta q_1 q_2\right)}. \tag{E.443}
$$

Note that (E.442) is equal to

$$\frac{1}{2}\int dq_1 dq_2\ (q_1^2+q_2^2)e^{-\frac{1}{2}\left(\alpha(q_1^2+q_2^2)+2\beta q_1 q_2\right)}. \tag{E.444}$$

If we define

$$I_0(\alpha,\beta)=\int dq_1 dq_2\ e^{-\frac{1}{2}\left(\alpha(q_1^2+q_2^2)+2\beta q_1 q_2\right)} \tag{E.445}$$

then

$$I_1=-\frac{\partial}{\partial\alpha}I_0(\alpha,\beta), \qquad I_2=-\frac{\partial}{\partial\beta}I_0(\alpha,\beta). \tag{E.446}$$

It is easy to evaluate $I_0(\alpha,\beta)$:

$$\begin{aligned}
I_0(\alpha,\beta) &= \int dq_1 dq_2\ e^{-\frac{1}{2}\left(\alpha(q_1^2+q_2^2)+2\beta q_1 q_2\right)} \\
&= \int dq_1 dq_2\ e^{-\frac{\alpha}{2}\left((q_1^2+q_2^2)+2(\beta/\alpha)q_1 q_2\right)} \\
&= \int dq_1 e^{-\frac{\alpha}{2}q_1^2}\int dq_2\ e^{-\frac{\alpha}{2}\left(q_2^2+2(\beta/\alpha)q_1 q_2\right)} \\
&= \int dq_1 e^{-\frac{\alpha}{2}q_1^2}\int dq_2\ e^{-\frac{\alpha}{2}\left((q_2+q_1(\beta/\alpha))^2-q_1^2(\beta/\alpha)^2\right)} \\
&= \int dq_1 e^{-\frac{1}{2}\left(\frac{\alpha^2-\beta^2}{\alpha}\right)q_1^2}\int dq_2\ e^{-\frac{\alpha}{2}q_2^2} \\
&= \sqrt{\frac{2\pi\alpha}{\alpha^2-\beta^2}}\cdot\sqrt{\frac{2\pi}{\alpha}} \\
&= \frac{2\pi}{\sqrt{\alpha^2-\beta^2}}.
\end{aligned} \tag{E.447}$$

Inserting this into (E.446) we have

$$I_1=\frac{2\pi\alpha}{(\alpha^2-\beta^2)^{3/2}}, \qquad I_2=-\frac{2\pi\beta}{(\alpha^2-\beta^2)^{3/2}}. \tag{E.448}$$

As $\alpha=\frac{\omega_a+\omega_b+2\omega}{2}$ and $\beta=\frac{\omega_a-\omega_b}{2}$,

$$\begin{aligned}
\alpha^2-\beta^2 &= \frac{(\omega_a+\omega_b+2\omega)^2-(\omega_a-\omega_b)^2}{4} \\
&= \frac{(\omega_a+\omega_b)^2-(\omega_a-\omega_b)^2+4\omega(\omega_a+\omega_b)+4\omega^2}{4} \\
&= \omega^2+\omega(\omega_a+\omega_b)+\omega_a\omega_b
\end{aligned} \tag{E.449}$$

and

$$
\begin{aligned}
I_1 &= \frac{\pi(2\omega+\omega_a+\omega_b)}{(\omega^2+\omega(\omega_a+\omega_b)+\omega_a\omega_b)^{3/2}}, \\
I_2 &= -\frac{\pi(\omega_a-\omega_b)}{(\omega^2+\omega(\omega_a+\omega_b)+\omega_a\omega_b)^{3/2}}.
\end{aligned}
\tag{E.450}
$$

Then

$$
{}_{loc}<1|1>=\frac{1}{\pi}\omega(\omega_a\omega_b)^{\frac{1}{4}}\big((\sqrt{\omega_a}+\sqrt{\omega_b})I_1+(\sqrt{\omega_a}-\sqrt{\omega_b})I_2\big) \tag{E.451}
$$

Let us expand

$$
\begin{aligned}
\omega^2+\omega(\omega_a+\omega_b)+\omega_a\omega_b &= \omega^2+\omega\big((\omega^2+\lambda)^{1/2}+(\omega^2-\lambda)^{1/2}\big)+(\omega^4-\lambda^2)^{1/2} \\
&= \omega^2\left[1+\left(1+\frac{\lambda}{\omega^2}\right)^{1/2}+\left(1-\frac{\lambda}{\omega^2}\right)^{1/2}+\left(1-\frac{\lambda^2}{\omega^4}\right)^{1/2}\right] \\
&= (2\omega)^2\left[1-\frac{3}{16}\frac{\lambda^2}{\omega^4}+\mathcal{O}(\lambda^4)\right]
\end{aligned}
\tag{E.452}
$$

and thus

$$
\begin{aligned}
\big(\omega^2+\omega(\omega_a+\omega_b)+\omega_a\omega_b\big)^{-3/2} &= (2\omega)^{-3}\left[1-\frac{3}{16}\frac{\lambda^2}{\omega^4}+\mathcal{O}(\lambda^4)\right]^{-3/2} \\
&= (2\omega)^{-3}\left[1+\frac{9}{32}\frac{\lambda^2}{\omega^4}+\mathcal{O}(\lambda^4)\right].
\end{aligned}
\tag{E.453}
$$

As well

$$
2\omega+\omega_a+\omega_b=4\omega\left[1-\frac{1}{16}\frac{\lambda^2}{\omega^4}+\mathcal{O}(\lambda^4)\right] \tag{E.454}
$$

and

$$
\omega_a-\omega_b=\omega\left(\frac{1}{2}\frac{\lambda}{\omega^2}+\mathcal{O}(\lambda^3)\right). \tag{E.455}
$$

So that

$$
\begin{aligned}
I_1 &= \pi \times 4\omega \left[1 - \frac{1}{16}\frac{\lambda^2}{\omega^4} + \mathcal{O}(\lambda^4)\right] \times (2\omega)^{-3} \left[1 + \frac{9}{32}\frac{\lambda^2}{\omega^4} + \mathcal{O}(\lambda^4)\right] \\
&= \pi \frac{1}{2\omega^2} \left[1 + \frac{7}{32}\frac{\lambda^2}{\omega^4} + \mathcal{O}(\lambda^4)\right] \qquad \text{(E.456)}
\end{aligned}
$$

and

$$
\begin{aligned}
I_2 &= -\pi \times \omega \left[\frac{1}{2}\frac{\lambda}{\omega^2} + \mathcal{O}(\lambda^3)\right] \times (2\omega)^{-3} \left[1 + \frac{9}{32}\frac{\lambda^2}{\omega^4} + \mathcal{O}(\lambda^4)\right] \\
&= -\pi \frac{1}{\omega^2} \left[\frac{1}{16}\frac{\lambda}{\omega^2} + \mathcal{O}(\lambda^3)\right] \qquad \text{(E.457)}
\end{aligned}
$$

Putting it all together

$$
\begin{aligned}
{}_{loc} < 1|1 > &= \frac{1}{\pi}\omega(\omega_a\omega_b)^{\frac{1}{4}} \left\{(\sqrt{\omega_a} + \sqrt{\omega_b})I_1 + (\sqrt{\omega_a} - \sqrt{\omega_b})I_2\right\} \\
&= \frac{1}{\pi}\omega \times \sqrt{\omega}\left(1 - \frac{1}{8}\frac{\lambda^2}{\omega^4} + \mathcal{O}(\lambda^4)\right) \times \\
&\quad \left\{2\sqrt{\omega}\left(1 - \frac{3}{32}\frac{\lambda^2}{\omega^4} + \mathcal{O}(\lambda^4)\right) \times \pi \frac{1}{2\omega^2}\left[1 + \frac{7}{32}\frac{\lambda^2}{\omega^4} + \mathcal{O}(\lambda^4)\right] - \right. \\
&\quad \left. \sqrt{\omega}\left(\frac{1}{2}\frac{\lambda}{\omega^2} + \mathcal{O}(\lambda^3)\right) \times \pi \frac{1}{\omega^2}\left[\frac{1}{16}\frac{\lambda}{\omega^2} + \mathcal{O}(\lambda^3)\right]\right\} \\
&= \left(1 - \frac{1}{8}\frac{\lambda^2}{\omega^4} + \mathcal{O}(\lambda^4)\right) \times \left\{\left(1 + \frac{1}{8}\frac{\lambda^2}{\omega^4} + \mathcal{O}(\lambda^4)\right) - \left(\frac{1}{32}\frac{\lambda^2}{\omega^4} + \mathcal{O}(\lambda^4)\right)\right\} \\
&= 1 - \frac{1}{32}\frac{\lambda^2}{\omega^4} + \mathcal{O}(\lambda^4) \qquad \text{(E.458)}
\end{aligned}
$$

Factorising chain of four oscillators

Show that

$$
H_0 = \frac{1}{2}\sum_{i=1}^{4}(p_i^2 + q_i^2) + \lambda \sum_{i=1}^{3} q_i q_{i+1} \qquad \text{(E.459)}
$$

factorises to

$$
H_0 = \frac{1}{2}\sum_{a=1}^{4}(p_a^2 + \omega_a^2 Q_a^2). \qquad \text{(E.460)}
$$

Hint: Consider an eigenvector problem. Use the trig-identity:

$$2\cos x \sin y = \sin(y-x) + \sin(y+x). \tag{E.461}$$

Proof:

We wish to equate

$$\begin{aligned}
&\frac{1}{2}(q_1^2+q_2^2+q_3^2+q_4^2) + \lambda q_1 q_2 + \lambda q_2 q_3 + \lambda q_3 q_4 = \\
&= \frac{1}{2}(q_1,q_2,q_3,q_4)\begin{pmatrix} 1 & \lambda & 0 & 0 \\ \lambda & 1 & \lambda & 0 \\ 0 & \lambda & 1 & \lambda \\ 0 & 0 & \lambda & 1 \end{pmatrix}\begin{pmatrix} q_1 \\ q_2 \\ q_3 \\ q_4 \end{pmatrix} = \frac{1}{2}(Q_1,Q_2,Q_3,Q_4)\begin{pmatrix} \omega_1^2 & 0 & 0 & 0 \\ 0 & \omega_2^2 & 0 & 0 \\ 0 & 0 & \omega_3^2 & 0 \\ 0 & 0 & 0 & \omega_4^2 \end{pmatrix}\begin{pmatrix} Q_1 \\ Q_2 \\ Q_3 \\ Q_4 \end{pmatrix}
\end{aligned} \tag{E.462}$$

where the $\mathbf{Q} = (Q_a)$, $a = 1, \ldots, 4$.

We look at the eigenvector problem:

$$\begin{pmatrix} 1 & \lambda & 0 & 0 \\ \lambda & 1 & \lambda & 0 \\ 0 & \lambda & 1 & \lambda \\ 0 & 0 & \lambda & 1 \end{pmatrix}\begin{pmatrix} e_1^{(a)} \\ e_2^{(a)} \\ e_3^{(a)} \\ e_4^{(a)} \end{pmatrix} = \beta^{(a)} \begin{pmatrix} e_1^{(a)} \\ e_2^{(a)} \\ e_3^{(a)} \\ e_4^{(a)} \end{pmatrix} \tag{E.463}$$

From the trig-identity:

$$2\cos x \sin y = \sin(y-x) + \sin(y+x) \tag{E.464}$$

we have:

$$\begin{aligned}
\lambda \sin\left(\frac{0\times a\pi}{5}\right) + \sin\left(\frac{a\pi}{5}\right) + \lambda\sin\left(\frac{2a\pi}{5}\right) &= \left(1+2\lambda\cos\left(\frac{a\pi}{5}\right)\right)\sin\left(\frac{a\pi}{5}\right) \\
\lambda \sin\left(\frac{a\pi}{5}\right) + \sin\left(\frac{2a\pi}{5}\right) + \lambda\sin\left(\frac{3a\pi}{5}\right) &= \left(1+2\lambda\cos\left(\frac{a\pi}{5}\right)\right)\sin\left(\frac{2a\pi}{5}\right) \\
\lambda \sin\left(\frac{2a\pi}{5}\right) + \sin\left(\frac{3a\pi}{5}\right) + \lambda\sin\left(\frac{4a\pi}{5}\right) &= \left(1+2\lambda\cos\left(\frac{a\pi}{5}\right)\right)\sin\left(\frac{3a\pi}{5}\right) \\
\lambda \sin\left(\frac{3a\pi}{5}\right) + \sin\left(\frac{4a\pi}{5}\right) + \lambda\sin\left(\frac{5a\pi}{5}\right) &= \left(1+2\lambda\cos\left(\frac{a\pi}{5}\right)\right)\sin\left(\frac{4a\pi}{5}\right)
\end{aligned} \tag{E.465}$$

where $a = 1, 2, 3, 4$. From which we see the eigenvector problem, (E.463), is solved for

$$e_i^{(a)} = C_{(4)} \sin\left(\frac{ia\pi}{4+1}\right) \tag{E.466}$$

with eigenvalue:

$$\beta^{(a)} = 1 + 2\lambda \cos\left(\frac{a\pi}{4+1}\right). \tag{E.467}$$

We define a scalar product by $\mathbf{e}^{(b)T}\mathbf{e}^{(a)} = \sum_i e_i^{(b)} e_i^{(a)}$. Obviously, $\mathbf{e}^{(a)T}\mathbf{e}^{(a)} > 0$. It is easy to prove that, because the eigenvalues are distinct, that the eigenvectors $\mathbf{e}^{(a)}$ are orthogonal; denote the matrix in (E.463) by M. First we have

$$\mathbf{e}^{(b)T} M \mathbf{e}^{(a)} = \beta^{(a)} \mathbf{e}^{(b)T}\mathbf{e}^{(a)}. \tag{E.468}$$

Since the matrix M is symmetric the LHS can also be written as

$$\begin{aligned}
(\mathbf{e}^{(b)T} M \mathbf{e}^{(a)})^{TT} &= (\mathbf{e}^{(a)T} M^T \mathbf{e}^{(b)})^T \\
&= (\mathbf{e}^{(a)T} M \mathbf{e}^{(b)})^T \\
&= (\beta^{(b)} \mathbf{e}^{(a)T} \mathbf{e}^{(b)})^T \\
&= \beta^{(b)} \mathbf{e}^{(b)T} \mathbf{e}^{(a)}.
\end{aligned} \tag{E.469}$$

The difference between the last two equations is

$$0 = (\beta^{(a)} - \beta^{(b)}) \mathbf{e}^{(b)T}\mathbf{e}^{(a)}. \tag{E.470}$$

Thus,

$$\mathbf{e}^{(b)T}\mathbf{e}^{(a)} = 0 \quad \text{if} \quad a \neq b. \tag{E.471}$$

which is what we wished to establish.

We need to normalise $e_i^{(a)}$:

$$
\begin{aligned}
1 &= \sum_{j=1}^{4} e_j^{(a)} e_j^{(a)} \\
&= C_{(4)}^2 \sum_{j=1}^{4} \sin^2\left(\frac{\pi a j}{4+1}\right) \\
&= C_{(4)}^2 \frac{1}{2} \sum_{j=1}^{4} \left(1 - \cos\left(\frac{2\pi a j}{4+1}\right)\right) \\
&= C_{(4)}^2 \left(\frac{4}{2} - \frac{1}{4}\sum_{j=1}^{4} \exp\left(i\frac{2\pi a j}{4+1}\right) - \frac{1}{4}\sum_{j=1}^{4} \exp\left(-i\frac{2\pi a j}{4+1}\right)\right) \\
&= C_{(4)}^2 \left(\frac{4}{2} - \frac{1}{4}\frac{\exp\left(i\frac{2\pi a}{4+1}\right) - \exp\left(i\frac{2\pi a(4+1)}{4+1}\right)}{1-\exp\left(i\frac{2\pi a}{4+1}\right)} - \frac{1}{4}\frac{\exp\left(-i\frac{2\pi a}{4+1}\right) - \exp\left(-i\frac{2\pi a(4+1)}{4+1}\right)}{1-\exp\left(-i\frac{2\pi a}{4+1}\right)}\right) \\
&= C_{(4)}^2 \left(\frac{4}{2} - \frac{1}{4}\frac{\exp\left(i\frac{2\pi a}{4+1}\right) - 1}{1-\exp\left(i\frac{2\pi a}{4+1}\right)} - \frac{1}{4}\frac{\exp\left(-i\frac{2\pi a}{4+1}\right) - 1}{1-\exp\left(-i\frac{2\pi a}{4+1}\right)}\right) \\
&= C_{(4)}^2 \frac{4+1}{2}. \qquad \text{(E.472)}
\end{aligned}
$$

Therefore we have

$$
e_i^{(a)} = \sqrt{\frac{2}{4+1}} \sin\left(\frac{ia\pi}{4+1}\right). \qquad \text{(E.473)}
$$

Construction of the orthogonal matrix:

$$
\begin{aligned}
(U_{ia}^{(4)T}) &:= \begin{pmatrix} e_1^{(1)} & e_1^{(2)} & e_1^{(3)} & e_1^{(4)} \\ e_2^{(1)} & e_2^{(2)} & e_2^{(3)} & e_2^{(4)} \\ e_3^{(1)} & e_3^{(2)} & e_3^{(3)} & e_3^{(4)} \\ e_4^{(1)} & e_4^{(2)} & e_4^{(3)} & e_4^{(4)} \end{pmatrix} \\
&= (e_i^{(a)}). \qquad \text{(E.474)}
\end{aligned}
$$

We have $(U_{ai}^{(4)})(U_{ib}^{(4)T}) = \mathbf{e}^{(a)T}\mathbf{e}^{(b)} = \delta_{ab}$.

Write

$$
(D_{ab}) = \begin{pmatrix} \omega_1^2 & 0 & 0 & 0 \\ 0 & \omega_2^2 & 0 & 0 \\ 0 & 0 & \omega_3^2 & 0 \\ 0 & 0 & 0 & \omega_4^2 \end{pmatrix} = \begin{pmatrix} \beta^{(1)} & 0 & 0 & 0 \\ 0 & \beta^{(2)} & 0 & 0 \\ 0 & 0 & \beta^{(3)} & 0 \\ 0 & 0 & 0 & \beta^{(4)} \end{pmatrix}. \qquad \text{(E.475)}
$$

We have

$$\begin{aligned} Q_a D_{ab} Q_b &= Q_a (U^{(4)}_{ai}) M_{ij} (U^{(4)}_{jb}) Q_b \\ &= q_i M_{ij} q_j \end{aligned} \tag{E.476}$$

giving the original equation (E.462), implying $q_i = (U^{(4)}_{ib}) Q_b$ or $(U^{(4)})_{ai} q_i = (U^{(4)}_{ai})(U^{(4)}_{ib}) Q_b = \delta_{ab} Q_b = Q_a$.

Thus the normal coordinates are given by

$$Q_a = U^{(4)}_{ai} q_i, \tag{E.477}$$

with the normal frequencies

$$\omega_a = \sqrt{1 + 2\lambda \cos\theta_a}, \quad \text{where} \quad \theta_a = \frac{a\pi}{4+1}, \quad \text{and} \quad a = 1, \ldots, 4. \tag{E.478}$$

Chain of oscillators

(a) Diagonilisation of the hamiltonian.

The hamiltonian

$$H = \frac{1}{2}(|\mathbf{p}|^2 + |\mathbf{q}|^2) + \lambda \sum_{i=1}^{n-1} q^i q^{i+1} \tag{E.479}$$

where $|\mathbf{q}|^2 = \sum_i (q^i)^2$ is diagonalised in the coordinates $\mathbf{Q} = U^{(n)}\mathbf{q}$, where $U^{(n)}$ is an orthogonal $n \times n$ matrix

$$U^{(n)}_{ai} = \sqrt{\frac{2}{n+1}} \sin\left(\frac{ai\pi}{n+1}\right) \tag{E.480}$$

with normal frequencies

$$\omega_a = \sqrt{1 + 2\lambda \cos\theta_a}, \quad \text{where} \quad \theta_a = \frac{a\pi}{n+1}, \quad \text{and} \quad a = 1, 2, \ldots, n. \tag{E.481}$$

(b) The vacuum state.

Prove that the vacuum state is

$$< \mathbf{q}|0 >= \prod_{a=1}^{n} \left(\frac{\omega_a}{\pi}\right)^{1/4} e^{-\frac{1}{2}q^i D_{ij}^{(n)} q^j} \tag{E.482}$$

where

$$D_{ij}^{(n)} = \sum_a U_{ai}^{(n)} \omega_a U_{aj}^{(n)}. \tag{E.483}$$

proof:

Part (a)

$$\begin{aligned}
p_i &= -i\hbar \frac{\partial}{\partial q^i} \\
&= -i\hbar \sum_a \frac{\partial Q_a}{\partial q^i} \frac{\partial}{\partial Q_a} \\
&= -i\hbar \sum_a \frac{\partial (\sum_j U_{aj}^{(n)} q^j)}{\partial q^i} \frac{\partial}{\partial Q_a} \\
&= -i\hbar \sum_a U_{ai}^{(n)} \frac{\partial}{\partial Q_a}
\end{aligned} \tag{E.484}$$

$$\begin{aligned}
\sum_{i=1}^{n} (p_i)^2 &= -\hbar^2 \sum_{i=1}^{n} \left(\sum_a U_{ai}^{(n)} \frac{\partial}{\partial Q_a} \right)^2 \\
&= -\hbar^2 \sum_{a,b} \left(\sum_{i=1}^{n} U_{ai}^{(n)} U_{bi}^{(n)} \right) \frac{\partial}{\partial Q_a} \frac{\partial}{\partial Q_b} \\
&\equiv \sum_{a=1}^{n} (P_a)^2
\end{aligned} \tag{E.485}$$

implying $\sum_{i=1}^{n} U_{ai}^{(n)} U_{bi}^{(n)} = \delta_{ab}$ or

$$\sum_{i=1}^{n} U_{ai}^{(n)} (U^{(n)T})_{ib} = \delta_{ab}. \tag{E.486}$$

We remind a bit of matrix properties...if matrices $\mathbf{A}$ and $\mathbf{B}$ are square matices such that $\mathbf{AB}$ is non-singular then $\det(\mathbf{AB}) = \det \mathbf{A} \det \mathbf{B} \neq 0$, implying $\det \mathbf{A} \neq 0$ and $\det \mathbf{B} \neq 0$, meaning $\mathbf{A}$ and $\mathbf{B}$ are both non-singular. If $\mathbf{A}$ and $\mathbf{B}$ are square matrices such that $\mathbf{AB} = \mathbb{1}$ then $\mathbf{A} = \mathbf{B}^{-1}$ and $\mathbf{B} = \mathbf{A}^{-1}$; if $\mathbf{BA} = \mathbb{1}$ then $\mathbf{AB}$ is non-singular and hence $\mathbf{A}$ and $\mathbf{B}$ are both non-singular, and hence both invertible. Now multiply the equation $\mathbf{AB} = \mathbb{1}$ on the left by $\mathbf{A}^{-1}$

$$
\begin{aligned}
\mathbf{A}^{-1}(\mathbf{AB}) &= \mathbf{A}^{-1}\mathbb{1} \\
(\mathbf{A}^{-1}\mathbf{A})\mathbf{B} &= \mathbf{A}^{-1} \\
\mathbf{B} &= \mathbf{A}^{-1}
\end{aligned} \tag{E.487}
$$

Similarly, we can find $\mathbf{A} = \mathbf{B}^{-1}$.

Implying

$$
(U^{(n)T})_{ia} = ((U^{(n)})^{-1})_{ia}. \tag{E.488}
$$

Which means

$$
\sum_a ((U^{(n)})^{-1})_{ia} U_{aj} = \delta_{ij}. \tag{E.489}
$$

Now turn to...

$$
\begin{aligned}
\sum_{a=1}^{n} \omega_a^2 (Q_a)^2 &= \sum_{a=1}^{n} \omega_a^2 \left(\sum_{i=1}^{n} U_{ai}^{(n)} q^i \right)^2 \\
&= \sum_{i,j=1}^{n} \left(\sum_{a=1}^{n} \omega_a^2 U_{ai}^{(n)} U_{aj}^{(n)} \right) q^i q^j \\
&\equiv \sum_{i=1}^{n} (q^i)^2 + \lambda \sum_{i=1}^{n-1} q^i q^{i+1}
\end{aligned} \tag{E.490}
$$

We require

$$
(q_1, q_2, q_3, q_4, \cdots, q_{n-1}, q_n) \begin{pmatrix} 1 & \lambda & 0 & 0 & \cdots & 0 & 0 \\ \lambda & 1 & \lambda & 0 & \cdots & 0 & 0 \\ 0 & \lambda & 1 & \lambda & \cdots & 0 & 0 \\ 0 & 0 & \lambda & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 & \lambda \\ 0 & 0 & 0 & 0 & \cdots & \lambda & 1 \end{pmatrix} \begin{pmatrix} q_1 \\ q_2 \\ q_3 \\ q_4 \\ \vdots \\ q_{n-1} \\ q_n \end{pmatrix}
$$

$$
= (Q_1, Q_2, Q_3, Q_4, \cdots, Q_{n-1}, Q_n) \begin{pmatrix} \omega_1^2 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & \omega_2^2 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \omega_3^2 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \omega_4^2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & \omega_{n-1}^2 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & \omega_n^2 \end{pmatrix} \begin{pmatrix} Q_1 \\ Q_2 \\ Q_3 \\ Q_4 \\ \vdots \\ Q_{n-1} \\ Q_n \end{pmatrix} \tag{E.491}
$$

where $Q_a = U^{(n)}_{ai} q^i$. We are led to the eigenvector problem:

$$
\begin{pmatrix} 1 & \lambda & 0 & 0 & \cdots & 0 & 0 \\ \lambda & 1 & \lambda & 0 & \cdots & 0 & 0 \\ 0 & \lambda & 1 & \lambda & \cdots & 0 & 0 \\ 0 & 0 & \lambda & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 & \lambda \\ 0 & 0 & 0 & 0 & \cdots & \lambda & 1 \end{pmatrix} \begin{pmatrix} e_1^a \\ e_2^a \\ e_3^a \\ e_4^a \\ \vdots \\ e_{n-1}^a \\ e_n^a \end{pmatrix} = \beta^a \begin{pmatrix} e_1^a \\ e_2^a \\ e_3^a \\ e_4^a \\ \vdots \\ e_{n-1}^a \\ e_n^a \end{pmatrix} \tag{E.492}
$$

From the trig-identity:

$$
2 \cos x \sin y = \sin(y - x) + \sin(y + x) \tag{E.493}
$$

we have:

$$
\begin{aligned}
\lambda\sin\left(\frac{0\times a\pi}{n+1}\right)+\sin\left(\frac{a\pi}{n+1}\right)+\lambda\sin\left(\frac{2a\pi}{n+1}\right) &= \left(1+2\lambda\cos\left(\frac{a\pi}{n+1}\right)\right)\sin\left(\frac{a\pi}{n+1}\right)\\
\lambda\sin\left(\frac{a\pi}{n+1}\right)+\sin\left(\frac{2a\pi}{n+1}\right)+\lambda\sin\left(\frac{3a\pi}{n+1}\right) &= \left(1+2\lambda\cos\left(\frac{a\pi}{n+1}\right)\right)\sin\left(\frac{2a\pi}{n+1}\right)\\
\lambda\sin\left(\frac{2a\pi}{n+1}\right)+\sin\left(\frac{3a\pi}{n+1}\right)+\lambda\sin\left(\frac{4a\pi}{n+1}\right) &= \left(1+2\lambda\cos\left(\frac{a\pi}{n+1}\right)\right)\sin\left(\frac{3a\pi}{n+1}\right)\\
\lambda\sin\left(\frac{3a\pi}{n+1}\right)+\sin\left(\frac{4a\pi}{n+1}\right)+\lambda\sin\left(\frac{5a\pi}{n+1}\right) &= \left(1+2\lambda\cos\left(\frac{a\pi}{n+1}\right)\right)\sin\left(\frac{4a\pi}{n+1}\right)\\
\vdots &= \vdots\\
\lambda\sin\left(\frac{(n-1)a\pi}{n+1}\right)+\sin\left(\frac{na\pi}{n+1}\right)+\lambda\sin\left(\frac{(n+1)a\pi}{n+1}\right) &= \left(1+2\lambda\cos\left(\frac{a\pi}{n+1}\right)\right)\sin\left(\frac{na\pi}{n+1}\right)
\end{aligned}
\tag{E.494}
$$

where $a = 1, 2, \ldots, n$. From which we see the eigenvectors are

$$
e_i^{(a)} = C_{(n)} \sin\left(\frac{ia\pi}{n+1}\right) \tag{E.495}
$$

where the eigenvalues are

$$
\beta^{(a)} = 1 + 2\lambda\cos\left(\frac{a\pi}{n+1}\right). \tag{E.496}
$$

As these eigenvalues are distinct, we have

$$
\mathbf{e}^{(b)T}\mathbf{e}^{(a)} = 0 \qquad \text{for} \quad a \neq b. \tag{E.497}
$$

We need the $e_i^{(a)}$ to be normalised:

$$
\begin{aligned}
1 &= \sum_{j=1}^{n} e_j^{(a)} e_j^{(a)} \\
&= C_{(n)}^2 \sum_{j=1}^{n} \sin^2\left(\frac{\pi a j}{n+1}\right) \\
&= C_{(n)}^2 \frac{1}{2} \sum_{j=1}^{n} \left(1 - \cos\left(\frac{2\pi a j}{n+1}\right)\right) \\
&= C_{(n)}^2 \left(\frac{n}{2} - \frac{1}{4}\sum_{j=1}^{n} \exp\left(i\frac{2\pi a j}{n+1}\right) - \frac{1}{4}\sum_{j=1}^{n} \exp\left(-i\frac{2\pi a j}{n+1}\right)\right) \\
&= C_{(n)}^2 \left(\frac{n}{2} - \frac{1}{4}\frac{\exp\left(i\frac{2\pi a}{n+1}\right) - \exp\left(i\frac{2\pi a(n+1)}{n+1}\right)}{1-\exp\left(i\frac{2\pi a}{n+1}\right)} - \frac{1}{4}\frac{\exp\left(-i\frac{2\pi a}{n+1}\right) - \exp\left(-i\frac{2\pi a(n+1)}{n+1}\right)}{1-\exp\left(-i\frac{2\pi a}{n+1}\right)}\right) \\
&= C_{(n)}^2 \left(\frac{n}{2} - \frac{1}{4}\frac{\exp\left(i\frac{2\pi a}{n+1}\right) - 1}{1-\exp\left(i\frac{2\pi a}{n+1}\right)} - \frac{1}{4}\frac{\exp\left(-i\frac{2\pi a}{n+1}\right) - 1}{1-\exp\left(-i\frac{2\pi a}{n+1}\right)}\right) \\
&= C_{(n)}^2 \frac{n+1}{2}.
\end{aligned}
\tag{E.498}
$$

Therefore we have

$$
e_i^{(a)} = \sqrt{\frac{2}{n+1}} \sin\left(\frac{i a \pi}{n+1}\right). \tag{E.499}
$$

Construction of the orthogonal matrix:

$$
\begin{aligned}
(U_{ia}^{(n)T}) &:= \begin{pmatrix}
e_1^{(1)} & e_1^{(2)} & e_1^{(3)} & e_1^{(4)} & \cdots & e_1^{(n-1)} & e_1^{(n)} \\
e_2^{(1)} & e_2^{(2)} & e_2^{(3)} & e_2^{(4)} & \cdots & e_2^{(n-1)} & e_2^{(n)} \\
e_3^{(1)} & e_3^{(2)} & e_3^{(3)} & e_3^{(4)} & \cdots & e_3^{(n-1)} & e_3^{(n)} \\
e_4^{(1)} & e_4^{(2)} & e_4^{(3)} & e_4^{(4)} & \cdots & e_4^{(n-1)} & e_4^{(n)} \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
e_{n-1}^{(1)} & e_{n-1}^{(2)} & e_{n-1}^{(3)} & e_{n-1}^{(4)} & \cdots & e_{n-1}^{(n-1)} & e_{n-1}^{(n)} \\
e_n^{(1)} & e_n^{(2)} & e_n^{(3)} & e_n^{(4)} & \cdots & e_n^{(n-1)} & e_n^{(n)}
\end{pmatrix} \\
&= (e_i^{(a)}).
\end{aligned}
\tag{E.500}
$$

From (E.497) and $\mathbf{e}^{(a)T}\mathbf{e}^{(a)} = 1$ for all a, we have

$$
\sum_i U_{ai}^{(n)} (U_{ia}^{(n)T}) = \delta_{ab}. \tag{E.501}
$$

(b) The vacuum state

$$\psi_0(Q) = \prod_{a=1}^{n} \left(\frac{\omega_a}{\pi}\right)^{1/4} e^{-\frac{1}{2}\sum_a \omega_a Q_a^2} \tag{E.502}$$

but

$$\begin{aligned}\sum_a \omega_a Q_a^2 &= \sum_a \omega_a \left(U_{ai}^{(n)} q^i\right)^2 \\ &= \sum_a q^i \left(U_{ai}^{(n)} \omega_a U_{aj}^{(n)}\right) q^j .\end{aligned} \tag{E.503}$$

Gaussian integral with source

If the matrix A is symmetric and strictly positive, prove that

$$\int \prod_{i=1}^{n} dx_i \exp\left(-\frac{1}{2}x^T A x + J^T x\right) = \left(\det\left(\frac{A}{2\pi}\right)\right)^{-1/2} \exp\left(\frac{1}{2}J^T A^{-1} J\right) \tag{E.504}$$

where $x^T A x = \sum_{i,j=1}^{n} x_i A_{ij} x_j$ and $J^T x = \sum_{i=1}^{n} J_i x_i$

Proof:

Make a change of variables

$$x = x' + A^{-1}J \tag{E.505}$$

then

$$-\frac{1}{2}x^T A x + J^T x = -\frac{1}{2}x'^T A x' + \frac{1}{2}J^T A^{-1} J \tag{E.506}$$

and

$$\int \prod_{i=1}^{n} dx_i \exp\left(-\frac{1}{2}x^T A x + J^T x\right) = \int \prod_{i=1}^{n} dx_i \exp\left(-\frac{1}{2}x^T A x\right) \exp\left(\frac{1}{2}J^T A^{-1} J\right). \tag{E.507}$$

We need to evaluate the integral

$$\int \prod_{i=1}^{n} dx_i \exp\left(-\frac{1}{2}x^T A x\right). \tag{E.508}$$

Let O be an orthogonal transformation ($OO^T = \mathbb{1}$) diagonalising A:

$$A = O^T D O, \qquad D = \begin{pmatrix} d_1 & & & \\ & d_1 & & 0 \\ 0 & & \ddots & \\ & & & d_n \end{pmatrix}, \qquad d_i > 0 \quad \text{for all } i. \tag{E.509}$$

Make the following change of variables with unit Jacobian:

$$x' = Ox \qquad (\det O = 1), \tag{E.510}$$

then

$$\int \prod_{i=1}^{n} dx_i \exp\left(-\frac{1}{2}x^T A x\right) = \int \prod_{i=1}^{n} dx'_i \exp\left(-\frac{1}{2}x'^T D x'\right). \tag{E.511}$$

The integral is the product of n independent gaussian integrals, and is given by

$$(2\pi)^{2/n} \prod_{i=1}^{n} d_i = \left(\det\left(\frac{A}{2\pi}\right)\right)^{-1/2}. \tag{E.512}$$

Thus

$$\int \prod_{i=1}^{n} dx_i \exp\left(-\frac{1}{2}x^T A x + J^T x\right) = \left(\det\left(\frac{A}{2\pi}\right)\right)^{-1/2} \exp\left(\frac{1}{2}J^T A^{-1} J\right). \tag{E.513}$$

Note that this implies:

$$\int \prod_{i=1}^{n} dx_i \exp\left(-x^T M x + J^T x\right) = \left(\det\left(\frac{M}{\pi}\right)\right)^{-1/2} \exp\left(\frac{1}{4}J^T M^{-1} J\right). \tag{E.514}$$

Expansions in λ

Establish the following expansions in λ:

$$
\begin{aligned}
\prod_{a=1}^{n_1} \sqrt{\tilde{\omega}_a} &\approx 1 - \lambda^2 \frac{n_1 - 1}{4} && \text{(E.515)} \\
\left(\det\left(\frac{A}{2}\right)\right)^{-1} &\approx 1 + \lambda^2 \left(\frac{n_1}{2} - \frac{7}{16}\right) && \text{(E.516)} \\
\left(\det\left(\frac{B}{2}\right)\right)^{-1/2} &\approx 1 + \lambda^2 \left(\frac{n_1}{4} - \frac{1}{8}\right) && \text{(E.517)}
\end{aligned}
$$

Hint:

$$
\begin{aligned}
\det\left(\mathbb{1} + h\right) &= \exp\left\{\ln\det\left(\mathbb{1} + h\right)\right\} \\
&= \exp\left\{\mathrm{tr}\ln\left(\mathbb{1} + h\right)\right\} \\
&= \exp\left\{\mathrm{tr}\left(h - \frac{h^2}{2} + \mathcal{O}(h^3)\right)\right\} \\
&= \exp\left\{\left(\mathrm{tr}h - \frac{1}{2}\mathrm{tr}h^2 + \mathcal{O}(h^3)\right)\right\}. && \text{(E.518)}
\end{aligned}
$$

Proof:

Part (a) Expression (E.515).

$$
\begin{aligned}
\prod_{a=1}^{n_1} \sqrt{\tilde{\omega}_a} &= \prod_{a=1}^{n_1} \left(1 + 2\lambda\cos\left(\frac{a\pi}{n_1+1}\right)\right)^{1/4} \\
&= \prod_{a=1}^{n_1} \left(1 + \frac{\lambda}{2}\cos\left(\frac{a\pi}{n_1+1}\right) - \frac{3}{8}\lambda^2\cos^2\left(\frac{a\pi}{n_1+1}\right) + \mathcal{O}(\lambda^3)\right) \\
&= 1 + \frac{\lambda}{2}\sum_{a=1}^{n_1}\cos\left(\frac{a\pi}{n_1+1}\right) + \frac{\lambda^2}{4}\sum_{a<b=1}^{n_1}\cos\left(\frac{a\pi}{n_1+1}\right)\cos\left(\frac{b\pi}{n_1+1}\right) \\
&\quad -\frac{3}{8}\lambda^2\sum_{a=1}^{n_1}\cos^2\left(\frac{a\pi}{n_1+1}\right) + \mathcal{O}(\lambda^3) && \text{(E.519)}
\end{aligned}
$$

Let us take each term at a time

$$
\begin{aligned}
\frac{\lambda}{2}\sum_{a=1}^{n_1}\cos\left(\frac{a\pi}{n_1+1}\right) &= \frac{\lambda}{4}\left(\sum_{a=1}^{n_1}\exp\left(i\frac{a\pi}{n_1+1}\right) + \sum_{a=1}^{n_1}\exp\left(-i\frac{a\pi}{n_1+1}\right)\right) \\
&= \frac{\lambda}{4}\left(\frac{\exp\left(i\frac{\pi}{n_1+1}\right)+1}{1-\exp\left(i\frac{\pi}{n_1+1}\right)} + \frac{1+\exp\left(i\frac{\pi}{n_1+1}\right)}{\exp\left(i\frac{\pi}{n_1+1}\right)-1}\right) \\
&= 0. && \text{(E.520)}
\end{aligned}
$$

A result that should have been obvious. Next

$$
\begin{aligned}
&\frac{\lambda^2}{4}\sum_{a<b=1}^{n_1}\cos\left(\frac{a\pi}{n_1+1}\right)\cos\left(\frac{b\pi}{n_1+1}\right) = \\
&= \frac{1}{2}\frac{\lambda^2}{4}\sum_{a,b=1}^{n_1}\cos\left(\frac{a\pi}{n_1+1}\right)\cos\left(\frac{b\pi}{n_1+1}\right) - \frac{1}{2}\frac{\lambda^2}{4}\sum_{a=1}^{n_1}\cos^2\left(\frac{a\pi}{n_1+1}\right) \\
&= \frac{\lambda^2}{8}\sum_{a=1}^{n_1}\cos\left(\frac{a\pi}{n_1+1}\right)\sum_{b=1}^{n_1}\cos\left(\frac{b\pi}{n_1+1}\right) - \frac{1}{2}\frac{\lambda^2}{4}\sum_{a=1}^{n_1}\cos^2\left(\frac{a\pi}{n_1+1}\right) \\
&= -\frac{1}{2}\frac{\lambda^2}{4}\sum_{a=1}^{n_1}\cos^2\left(\frac{a\pi}{n_1+1}\right) \\
&= -\frac{\lambda^2}{16}\sum_{a=1}^{n_1}\left\{1+\cos\left(\frac{a2\pi}{n_1+1}\right)\right\} \\
&= -\frac{\lambda^2}{16}(n_1-1) \qquad \text{(E.521)}
\end{aligned}
$$

where we used (E.520), and a result from (E.498) in the last line. The last term in (E.519) is then

$$
-\frac{3}{8}\lambda^2\sum_{a=1}^{n_1}\cos^2\left(\frac{a\pi}{n_1+1}\right) = -\frac{3}{16}\lambda^2(n_1-1). \qquad \text{(E.522)}
$$

Therefore, putting these results together, we have

$$
\prod_{a=1}^{n_1}\sqrt{\tilde{\omega}_a} \approx 1-\lambda^2\frac{n_1-1}{4}. \qquad \text{(E.523)}
$$

Part (b) Expression (E.516).

$$
\begin{aligned}
D_{ij}^{(n_1)} &= \sum_{a=1}^{n_1}\sqrt{\frac{2}{n_1+2}}\sin\left(\frac{ai\pi}{n_1+1}\right)\sqrt{1+2\lambda\cos\left(\frac{a\pi}{n_1+1}\right)}\sqrt{\frac{2}{n_1+2}}\sin\left(\frac{aj\pi}{n_1+1}\right) \\
&= \frac{2}{n_1+2}\sum_{a=1}^{n_1}\sin\left(\frac{ai\pi}{n_1+1}\right)\sin\left(\frac{aj\pi}{n_1+1}\right) \\
&\quad +\frac{2}{n_1+2}\lambda\sum_{a=1}^{n_1}\sin\left(\frac{ai\pi}{n_1+1}\right)\cos\left(\frac{a\pi}{n_1+1}\right)\sin\left(\frac{aj\pi}{n_1+1}\right) \\
&\quad -\frac{2}{n_1+2}\frac{1}{2}\lambda^2\sum_{a=1}^{n_1}\sin\left(\frac{ai\pi}{n_1+1}\right)\cos^2\left(\frac{a\pi}{n_1+1}\right)\sin\left(\frac{aj\pi}{n_1+1}\right)+\mathcal{O}(\lambda^3). \qquad \text{(E.524)}
\end{aligned}
$$

First

$$\begin{aligned}\frac{2}{n_1+1}\sum_{a=1}^{n_1}\sin\left(\frac{ai\pi}{n_1+1}\right)\sin\left(\frac{aj\pi}{n_1+1}\right) &= \delta_{ij},\\ \frac{2}{n+1}\sum_{a=1}^{n}\sin\left(\frac{ai\pi}{n+1}\right)\sin\left(\frac{aj\pi}{n+1}\right) &= \delta_{ij}.\end{aligned} \tag{E.525}$$

So $D^{(n_1)} = \mathbb{1}_{n_1} + \mathcal{O}(\lambda)$. Also, $D^{(n)} = \mathbb{1} + \mathcal{O}(\lambda)$. We can write

$$D^{(n_1)} = \mathbb{1}_{n_1} + \lambda M^{(n_1)} - \frac{1}{2}\lambda^2 \tilde{M}^{(n_1)} + \mathcal{O}(\lambda^3), \tag{E.526}$$

$$D^{(n)} = \mathbb{1}_{n_1} + \lambda M^{(n_1)} - \frac{1}{2}\lambda^2 \tilde{M}^{(n_1)} + \mathcal{O}(\lambda^3) \tag{E.527}$$

(here in part (b) the $D^{(n)}$ is understood as a matrix whose indices $i, j = 1, \ldots, n_1$) where

$$M_{ij}^{(n_1)} = \frac{2}{n_1+1}\sum_{a=1}^{n_1}\sin\left(\frac{ai\pi}{n_1+1}\right)\cos\left(\frac{a\pi}{n_1+1}\right)\sin\left(\frac{aj\pi}{n_1+1}\right), \tag{E.528}$$

$$\tilde{M}_{ij}^{(n_1)} = \frac{2}{n_1+1}\sum_{a=1}^{n_1}\sin\left(\frac{ai\pi}{n_1+1}\right)\cos^2\left(\frac{a\pi}{n_1+1}\right)\sin\left(\frac{aj\pi}{n_1+1}\right), \tag{E.529}$$

$$M_{ij}^{(n)} = \frac{2}{n+1}\sum_{a=1}^{n}\sin\left(\frac{ai\pi}{n+1}\right)\cos\left(\frac{a\pi}{n+1}\right)\sin\left(\frac{aj\pi}{n+1}\right), \tag{E.530}$$

$$\tilde{M}_{ij}^{(n)} = \frac{2}{n+1}\sum_{a=1}^{n}\sin\left(\frac{ai\pi}{n+1}\right)\cos^2\left(\frac{a\pi}{n+1}\right)\sin\left(\frac{aj\pi}{n+1}\right). \tag{E.531}$$

From the definition of the matrix A, we have

$$\begin{aligned}\frac{A}{2} &= \frac{1}{2}(D^{(n_1)} + D^{(n)})\\ &= \mathbb{1}_{n_1} + \frac{1}{2}\lambda\left(M^{(n_1)} + M^{(n)}\right) - \frac{1}{4}\lambda^2\left(\tilde{M}^{(n_1)} + \tilde{M}^{(n)}\right) + \mathcal{O}(\lambda^3)\\ &=: (\mathbb{1}_{n_1} + h).\end{aligned} \tag{E.532}$$

A similar calculation to (E.518) gives

$$
\begin{aligned}
\left(\det\left(\frac{A}{2}\right)\right)^{-1} &= (\det(\mathbb{1}_{n_1}+h))^{-1} \\
&= \exp\left\{-\ln\det\left((\mathbb{1}_{n_1}+h)\right)\right\} \\
&= \exp\left\{-\mathrm{tr}_{n_1}\ln\left(\mathbb{1}_{n_1}+h\right)\right\} \\
&= \exp\left\{-\mathrm{tr}_{n_1}\left(h-\frac{h^2}{2}+\mathcal{O}(h^3)\right)\right\} \\
&= \exp\left\{-\mathrm{tr}_{n_1}h+\frac{1}{2}\mathrm{tr}_{n_1}h^2+\mathcal{O}(h^3)\right\} \\
&= \left(\mathbb{1}_{n_1}-\mathrm{tr}_{n_1}h+\frac{1}{2}\mathrm{tr}_{n_1}h^2+\frac{1}{2!}(\mathrm{tr}_{n_1}h)^2+\mathcal{O}(h^3)\right).
\end{aligned}
\tag{E.533}
$$

The matrix h defined in (E.532) is

$$
h=\frac{1}{2}\lambda\left(M^{(n_1)}+M^{(n)}\right)-\frac{1}{4}\lambda^2\left(\tilde{M}^{(n_1)}+\tilde{M}^{(n)}\right)+\mathcal{O}(\lambda^3). \tag{E.534}
$$

Inserting this expression for h into (E.533) we have

$$
\begin{aligned}
&\left(\det\left(\frac{A}{2}\right)\right)^{-1}=\left(1-\mathrm{tr}_{n_1}h+\frac{1}{2}\mathrm{tr}_{n_1}h^2+\frac{1}{2}(\mathrm{tr}_{n_1}h)^2+\mathcal{O}(h^3)\right)= \\
&=1-\frac{1}{2}\lambda\left(\mathrm{tr}_{n_1}M^{(n_1)}+\mathrm{tr}_{n_1}M^{(n)}\right)+\frac{1}{4}\lambda^2\left(\mathrm{tr}_{n_1}\tilde{M}^{(n_1)}+\mathrm{tr}_{n_1}\tilde{M}^{(n)}\right) \\
&+\frac{1}{8}\lambda^2\mathrm{tr}_{n_1}\left(M^{(n_1)}+M^{(n)}\right)^2+\frac{1}{8}\lambda^2\left(\mathrm{tr}_{n_1}M^{(n_1)}+\mathrm{tr}_{n_1}M^{(n)}\right)^2+\mathcal{O}(\lambda^3).
\end{aligned}
\tag{E.535}
$$

In the following (E.525) will be extensively employed.

First, from

$$
\begin{aligned}
M_{ij}^{(n_1)} &= \frac{2}{n_1+1}\sum_{a=1}^{n_1}\sin\left(\frac{ai\pi}{n_1+1}\right)\cos\left(\frac{a\pi}{n_1+1}\right)\sin\left(\frac{aj\pi}{n_1+1}\right) \\
&= \frac{1}{2}\frac{2}{n_1+1}\sum_{a=1}^{n_1}\sin\left(\frac{ai\pi}{n_1+1}\right)\left\{\sin\left(\frac{a(j-1)\pi}{n_1+1}\right)+sin\left(\frac{a(j+1)\pi}{n_1+1}\right)\right\} \\
&= \frac{1}{2}(\delta_{i,j-1}+\delta_{i,j+1})
\end{aligned}
\tag{E.536}
$$

we obviously have

$$\text{tr}_{n_1} M^{(n_1)} = 0. \tag{E.537}$$

Consider

$$\begin{aligned} M_{ij}^{(n)} &= \frac{2}{n+1}\sum_{a=1}^{n} \sin\left(\frac{ai\pi}{n+1}\right)\cos\left(\frac{a\pi}{n+1}\right)\sin\left(\frac{aj\pi}{n+1}\right) \\ &= \frac{1}{2}\frac{2}{n+1}\sum_{a=1}^{n} \sin\left(\frac{ai\pi}{n+1}\right)\left(\sin\left(\frac{a(j-1)\pi}{n+1}\right) + \sin\left(\frac{a(j+1)\pi}{n+1}\right)\right) \\ &= \frac{1}{2}(\delta_{i,j-1} + \delta_{i,j+1}) \end{aligned} \tag{E.538}$$

then

$$\text{tr}_{n_1} M^{(n)} = 0. \tag{E.539}$$

Substituting these results into (E.539) we see that $\text{tr}_{n_1} M^{(n)} = 0$. The expression (E.535) then simplifies to

$$\begin{aligned} \left(\det\left(\frac{A}{2}\right)\right)^{-1} &= 1 + \frac{1}{4}\lambda^2\left(\text{tr}_{n_1}\tilde{M}^{(n_1)} + \text{tr}_{n_1}\tilde{M}^{(n)}\right) \\ &\quad + \frac{1}{8}\lambda^2 \text{tr}_{n_1}\left(M^{(n_1)} + M^{(n)}\right)^2 + \mathcal{O}(\lambda^3). \end{aligned} \tag{E.540}$$

Now we turn to the matrices (E.530) and (E.531). We calculate

$$\begin{aligned} \tilde{M}_{ij}^{(n_1)} &= \frac{2}{n_1+1}\sum_{a=1}^{n_1} \sin\left(\frac{ai\pi}{n_1+1}\right)\cos^2\left(\frac{a\pi}{n_1+1}\right)\sin\left(\frac{aj\pi}{n_1+1}\right) \\ &= \frac{1}{2}\frac{2}{n_1+1}\sum_{a=1}^{n_1} \sin\left(\frac{ai\pi}{n_1+1}\right)\left\{1 + \cos\left(\frac{2a\pi}{n_1+1}\right)\right\}\sin\left(\frac{aj\pi}{n_1+1}\right) \\ &= \frac{1}{2}\frac{2}{n_1+1}\sum_{a=1}^{n_1} \sin\left(\frac{ai\pi}{n_1+1}\right)\sin\left(\frac{aj\pi}{n_1+1}\right) \\ &\quad + \frac{1}{4}\frac{2}{n_1+1}\sum_{a=1}^{n_1} \sin\left(\frac{ai\pi}{n_1+1}\right)\left\{\sin\left(\frac{a(j-2)\pi}{n_1+1}\right) + \sin\left(\frac{a(j+2)\pi}{n_1+1}\right)\right\} \\ &= \frac{1}{2}\delta_{i,j} + \frac{1}{4}(\delta_{i,j-2} + \delta_{i,j+2}) - \frac{1}{2}\delta_{i,1} \end{aligned} \tag{E.541}$$

so that

$$
\begin{aligned}
\mathrm{tr}_{n_1}\tilde{M}^{(n_1)} &= \sum_{i=1}^{n_1}(\frac{1}{2}\delta_{i,i}-\frac{1}{2}\delta_{i,1}) \\
&= \frac{1}{2}(n_1-1)
\end{aligned} \tag{E.542}
$$

Next

$$
\begin{aligned}
\tilde{M}^{(n)}_{ij} &= \frac{2}{n+1}\sum_{a=1}^{n}\sin\left(\frac{ai\pi}{n+1}\right)\cos^2\left(\frac{a\pi}{n+1}\right)\sin\left(\frac{aj\pi}{n+1}\right) \\
&= \frac{1}{2}\frac{2}{n+1}\sum_{a=1}^{n}\sin\left(\frac{ai\pi}{n+1}\right)\left\{1+\cos\left(\frac{2a\pi}{n+1}\right)\right\}\sin\left(\frac{aj\pi}{n+1}\right) \\
&= \frac{1}{2}\frac{2}{n+1}\sum_{a=1}^{n}\sin\left(\frac{ai\pi}{n+1}\right)\sin\left(\frac{aj\pi}{n+1}\right) \\
&\quad +\frac{1}{4}\frac{2}{n+1}\sum_{a=1}^{n}\sin\left(\frac{ai\pi}{n+1}\right)\left\{\sin\left(\frac{a(j-2)\pi}{n+1}\right)+\sin\left(\frac{a(j+2)\pi}{n+1}\right)\right\} \\
&= \frac{1}{2}\delta_{i,j}+\frac{1}{4}(\delta_{i,j-2}+\delta_{i,j+2})-\frac{1}{4}\delta_{i,1}
\end{aligned} \tag{E.543}
$$

so that

$$
\begin{aligned}
\mathrm{tr}_{n_1}\tilde{M}^{(n)} &= \sum_{i=1}^{n_1}(\frac{1}{2}\delta_{i,i}-\frac{1}{4}\delta_{i,1}) \\
&= \frac{1}{4}(2n_1-1).
\end{aligned} \tag{E.544}
$$

We easily see

$$
\begin{aligned}
((M^{(n_1)})^2)_{ij} &= \sum_{k=1}^{n_1}M^{(n_1)}_{ik}M^{(n_1)}_{kj} \\
&= \left(\frac{2}{n_1+1}\right)^2\sum_{a,b=1}^{n_1}\sin\left(\frac{ai\pi}{n_1+1}\right)\cos\left(\frac{a\pi}{n_1+1}\right)\sum_{k=1}^{n_1}\sin\left(\frac{ak\pi}{n_1+1}\right)\sin\left(\frac{bk\pi}{n_1+1}\right)\times \\
&\quad \times\cos\left(\frac{b\pi}{n_1+1}\right)\sin\left(\frac{bj\pi}{n_1+1}\right) \\
&= \frac{2}{n_1+1}\sum_{a=1}^{n_1}\sin\left(\frac{ai\pi}{n_1+1}\right)\cos^2\left(\frac{a\pi}{n_1+1}\right)\sin\left(\frac{aj\pi}{n_1+1}\right) \\
&= (\tilde{M}^{(n_1)})_{ij}
\end{aligned} \tag{E.545}
$$

and thus

$$\mathrm{tr}_{n_1}((M^{(n_1)})^2) = \mathrm{tr}_{n_1}\tilde{M}^{(n_1)} = \frac{1}{2}\,(n_1 - 1)\,. \tag{E.546}$$

Next

$$\begin{aligned}
((M^{(n)})^2)_{ij} &= \sum_{i=1}^{n_1}\sum_{k=1}^{n_1} M_{ik}^{(n)} M_{kj}^{(n)} \\
&= \sum_{k=1}^{n_1} \frac{2}{n+1} \sum_{a=1}^{n} \sin\left(\frac{ai\pi}{n+1}\right)\cos\left(\frac{a\pi}{n+1}\right)\sin\left(\frac{ak\pi}{n+1}\right) \times \\
&\quad \times \frac{2}{n+1} \sum_{b=1}^{n} \sin\left(\frac{bk\pi}{n+1}\right)\cos\left(\frac{b\pi}{n+1}\right)\sin\left(\frac{bj\pi}{n+1}\right) \\
&= \frac{1}{4}\sum_{k=1}^{n_1} \frac{2}{n+1} \sum_{a=1}^{n} \left\{\sin\left(\frac{a(i-1)\pi}{n+1}\right) + \sin\left(\frac{a(i+1)\pi}{n+1}\right)\right\}\sin\left(\frac{ak\pi}{n+1}\right) \times \\
&\quad \times \frac{2}{n+1} \sum_{b=1}^{n} \sin\left(\frac{bk\pi}{n+1}\right)\left\{\sin\left(\frac{b(j-1)\pi}{n+1}\right) + \sin\left(\frac{b(j+1)\pi}{n+1}\right)\right\} \\
&= \frac{1}{4}\sum_{k=1}^{n_1} (\delta_{i-1,k} + \delta_{i+1,k})(\delta_{k,j-1} + \delta_{k,j+1}) \\
&= \frac{1}{4}(\delta_{i-1,j-1} + \delta_{i-1,j+1} + \delta_{i+1,j-1} + \delta_{i+1,j+1})
\end{aligned} \tag{E.547}$$

so

$$\begin{aligned}
\mathrm{tr}_{n_1}((M^{(n)})^2) &= \frac{1}{4}\sum_{i=1}^{n_1} (\delta_{i-1,i-1} + \delta_{i-1,i+1} + \delta_{i+1,i-1} + \delta_{i+1,i+1}) \\
&= \frac{1}{2}(n_1 - 1).
\end{aligned} \tag{E.548}$$

Next

$$
\begin{aligned}
(M^{(n_1)}M^{(n)})_{ij} &= \sum_{k=1}^{n_1} M_{ik}^{(n_1)} M_{kj}^{(n)} \\
&= \sum_{k=1}^{n_1} \frac{2}{n_1+1} \sum_{a=1}^{n_1} \sin\left(\frac{ai\pi}{n_1+1}\right)\cos\left(\frac{a\pi}{n_1+1}\right)\sin\left(\frac{ak\pi}{n_1+1}\right) \times \\
&\quad \times \frac{2}{n+1}\sum_{b=1}^{n} \sin\left(\frac{bk\pi}{n+1}\right)\cos\left(\frac{b\pi}{n+1}\right)\sin\left(\frac{bj\pi}{n+1}\right) \\
&= \frac{1}{4}\sum_{k=1}^{n_1} \frac{2}{n_1+1}\sum_{a=1}^{n_1}\left\{\sin\left(\frac{a(i-1)\pi}{n_1+1}\right)+\sin\left(\frac{a(i+1)\pi}{n_1+1}\right)\right\}\sin\left(\frac{ak\pi}{n_1+1}\right) \times \\
&\quad \times \frac{2}{n+1}\sum_{b=1}^{n}\sin\left(\frac{bk\pi}{n+1}\right)\left\{\sin\left(\frac{b(j-1)\pi}{n+1}\right)+\sin\left(\frac{b(j+1)\pi}{n+1}\right)\right\} \\
&= \frac{1}{4}\sum_{k=1}^{n_1}(\delta_{i-1,k}+\delta_{i+1,k})(\delta_{k,j-1}+\delta_{k,j+1}) \\
&= \frac{1}{4}(\delta_{i-1,j-1}+\delta_{i-1,j+1}+\delta_{i+1,j-1}+\delta_{i+1,j+1}) \qquad \text{(E.549)}
\end{aligned}
$$

so

$$
\begin{aligned}
2\mathrm{tr}_{n_1}(M^{(n_1)})(M^{(n)}) &= 2\sum_{i=1}^{n_1}\sum_{k=1}^{n_1} M_{ik}^{(n_1)}M_{ki}^{(n)} \\
&= \frac{1}{2}\sum_{i=1}^{n_1}(\delta_{i-1,i-1}+\delta_{i-1,i+1}+\delta_{i+1,i-1}+\delta_{i+1,i+1}) \\
&= (n_1-1). \qquad \text{(E.550)}
\end{aligned}
$$

The expression (E.535) then gives

$$
\begin{aligned}
\left(\det\left(\frac{A}{2}\right)\right)^{-1} &= 1+\frac{1}{4}\lambda^2\left(\mathrm{tr}_{n_1}\tilde{M}^{(n_1)}+\mathrm{tr}_{n_1}\tilde{M}^{(n)}\right) \\
&\quad +\frac{1}{8}\lambda^2\left(\mathrm{tr}_{n_1}(M^{(n_1)})^2+2\mathrm{tr}_{n_1}(M^{(n)}M^{(n_1)})+\mathrm{tr}_{n_1}(M^{(n)})^2\right)+\mathcal{O}(\lambda^3) \\
&= 1+\frac{1}{4}\lambda^2\left(\frac{1}{2}(n_1-1)+\frac{1}{4}(2n_1-1)\right) \\
&\quad +\frac{1}{8}\lambda^2\left(\frac{1}{2}(n_1-1)+(n_1-1)+\frac{1}{2}(n_1-1)\right)+\mathcal{O}(\lambda^3) \\
&= 1+\lambda^2\left(\frac{n_1}{2}-\frac{7}{16}\right)+\mathcal{O}(\lambda^3). \qquad \text{(E.551)}
\end{aligned}
$$

Expansions in λ of correlation function.

Prove that

$$\left(D^{(n_1)}\right)^{-1}_{ij} \approx \left(1+\frac{3}{4}\lambda^2\right)\delta_{i,j} - \frac{1}{2}\lambda\delta_{i,j\pm 1} + \frac{3}{8}\lambda^2\delta_{i,j\pm 2} + \dots \tag{E.552}$$

Proof:

If $D^{(n_1)} = (\mathbb{1}_{n_1} + b)$ then

$$\begin{aligned} \left(D^{(n_1)}\right)^{-1} &= (\mathbb{1}_{n_1} + b)^{-1} \\ &= \mathbb{1}_{n_1} - b + b^2 - b^3 + \mathcal{O}(b^4). \end{aligned} \tag{E.553}$$

Recall

$$D^{(n_1)} = \mathbb{1}_{n_1} + \lambda M^{(n_1)} - \frac{1}{2}\lambda^2 \tilde{M}^{(n_1)} + \mathcal{O}(\lambda^3). \tag{E.554}$$

Substituting this into (E.553)

$$\begin{aligned} \left(D^{(n_1)}\right)^{-1}_{ij} &= (\mathbb{1}_{n_1} + b)^{-1}_{ij} \\ &= \delta_{i,j} - \left(\lambda M^{(n_1)}_{ij} - \frac{1}{2}\lambda^2 \tilde{M}^{(n_1)}_{ij}\right) + \lambda^2 \left(M^{(n_1)}\right)^2_{ij} + \mathcal{O}(\lambda^3) \\ &= \delta_{i,j} - \lambda\frac{1}{2}(\delta_{i,j-1} + \delta_{i,j-1}) + \frac{1}{2}\lambda^2\left(\frac{1}{2}\delta_{i,j} + \frac{1}{4}(\delta_{i,j-2} + \delta_{i,j+2}) - \frac{1}{2}\delta_{i,1}\right) \\ &\quad + \lambda^2\left(\frac{1}{2}\delta_{i,j} + \frac{1}{4}(\delta_{i,j-2} + \delta_{i,j+2}) - \frac{1}{2}\delta_{i,1}\right) + \mathcal{O}(\lambda^3) \\ &= \left(1+\frac{3}{4}\lambda^2\right)\delta_{i,j} - \frac{1}{2}\lambda(\delta_{i,j-1} + \delta_{i,j-1}) + \frac{3}{8}\lambda^2(\delta_{i,j-2} + \delta_{i,j+2}) - \frac{3}{4}\lambda^2\delta_{i,1} + \mathcal{O}(\lambda^3) \end{aligned} \tag{E.555}$$

where we have used (E.536), (E.541) and (E.545).