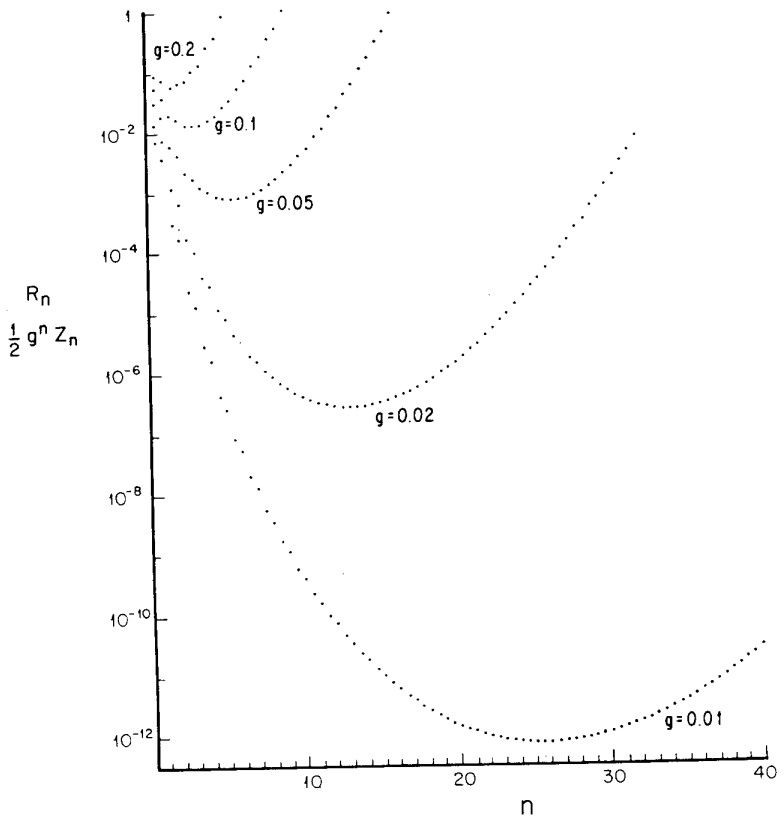

Fig. 2.2 Asymptotic expansion of $Z(g)$. For five values of the coupling constant, $\frac{1}{2}g^n|Z_n|$ is plotted at each integer n and the residual error R_n is plotted at each half integer $n + \frac{1}{2}$.

after only attaining an accuracy of 25%. If one wishes to do better, one must either extract the non-analytic part of $Z(g)$ using the Borel summation discussed in Section 7.5 or find an alternative expansion.

For other regimes of the potentials sketched in Fig. 2.1, other expansions are more appropriate than (2.26). For large positive g, it is more reasonable to make a strong coupling expansion by starting with the solution to the quartic potential and treating the quadratic potential as the perturbation. For case (c), the natural approach is the stationary phase approximation which will be discussed at length in Section 2.5. In this case, the partition function is written $\tilde{Z}(g) = \int \frac{dx}{\sqrt{2\pi}} e^{\frac{x^2}{2} - \frac{g}{4}x^4} = \int \frac{dy}{\sqrt{2\pi g}} e^{-\frac{1}{g}\left[-\frac{y^2}{2} + \frac{y^4}{4}\right]}$ and the exponent is expanded around its two maxima $y = \pm 1$ corresponding to the minimum of the potential.

The general features illustrated by the quadratic plus quartic potential are pertinent to the richer and more complicated case of the many-body problem. We will find that different approximations will address different aspects of the physics. Perturbation theory in the two-body interaction, while at best an asymptotic expansion, will serve to organize our thinking and elucidate much of the general structure of the problem. Various resummations will focus on different parts of the physics such as short-range or long-range correlations. The stationary phase approximation will address still other aspects of the problem such as large amplitude collective motion and tunnelling. In all of these expansions, there will be some formal expansion parameter which provides no real mathematical control on the problem. The most we can ask in practice, as in the example in Fig. 2.2, is that successive terms in the series of approximations decrease.

2.2 FUNCTIONAL INTEGRAL FORMULATION

Functional integrals provide a powerful tool for the study of many-particle systems. The partition function is represented by an integral over field configurations which provides both a physically intuitive description of the system and a useful starting point for approximations. Approximations which arise naturally from functional integrals include perturbation expansions, loop expansions around stationary solutions, approximations in terms of solitons or instantons, and stochastic approximations. Before proceeding to the general case of many-particle systems, it is instructive to illustrate the essential idea with Feynman path integrals. The essence of the path integral was introduced in a germinal paper by P.A.M. Dirac (1933) and developed extensively by R.P. Feynman (1948,1949,1950). All these historic papers are published in the reprint volume edited by J. Schwinger(1953).

THE FEYNMAN PATH INTEGRAL

For physical clarity, we will first introduce the Feynman path integral in real time. Subsequently, in order to represent the partition function, we shall perform an analytic continuation to imaginary time where this path integral is closely related to the Wiener integral and is mathematically well-defined.

Consider a matrix element of the evolution operator for a particle governed by the Hamiltonian $H(\hat{p}, \hat{x})$

$$\mathcal{U}(x_f t_f, x_i t_i) = \langle x_f | e^{-\frac{i}{\hbar}\hat{H}(t_f - t_i)} | x_i \rangle \quad . \tag{2.28}$$

Whereas the matrix elements of the evolution operator cannot be evaluated exactly for finite time intervals, for infinitesimal time intervals they may be calculated to any desired degree of accuracy. Thus, the basic idea of the Feynman path integral is to break a finite time interval into infinitesimal steps, evaluate the evolution operator for each step, and chain the matrix elements together to obtain the result for the finite interval.

Let the time interval $t_f - t_i$ be divided into M equal steps of size ϵ

$$\epsilon = \frac{t_f - t_i}{M} \tag{2.29a}$$

with intermediate times denoted

$$t_n = t_i + (n\epsilon) \epsilon \ . \tag{2.29b}$$

With this notation,

$$t_0 \equiv t_i \quad \text{and} \quad t_M \equiv t_f \tag{2.29c}$$

and it will be convenient to use the same convention for initial and final coordinates

$$x_0 \equiv x_i \quad \text{and} \quad x_M \equiv x_f \ . \tag{2.29d}$$

By inserting the closure relation Eq. (1.23) $M-1$ times, the matrix element of the evolution operator may be written:

$$\begin{aligned} U(x_f t_f, x_i t_i) &= \langle x_f | \left(e^{-i\frac{\epsilon}{\hbar}\hat{H}} \right)^M | x_i \rangle \\ &= \int \prod_{k=1}^{M-1} dx_k \langle x_f | e^{-i\frac{\epsilon}{\hbar}\hat{H}} | x_{M-1} \rangle \langle x_{M-1} | e^{-i\frac{\epsilon}{\hbar}\hat{H}} | x_{M-2} \rangle \\ &\quad \times \langle x_{M-2} | \ldots e^{-i\frac{\epsilon}{\hbar}\hat{H}} | x_1 \rangle \langle x_1 | e^{-i\frac{\epsilon}{\hbar}\hat{H}} | x_i \rangle \ . \end{aligned} \tag{2.30}$$

The key step is to find an appropriate approximation for the matrix element of the infinitesimal evolution operator, which may be written

$$\langle x_n | e^{-i\frac{\epsilon}{\hbar}H(\hat{p},\hat{x})} | x_{n-1} \rangle = \int d^3 p_n \langle x_n | p_n \rangle \langle p_n | e^{-i\frac{\epsilon}{\hbar}H(\hat{p},\hat{x})} | x_{n-1} \rangle \ . \tag{2.31}$$

For our purposes in obtaining a practical functional integral, we desire an approximation to the infinitesimal evolution operator $e^{-i\frac{\epsilon}{\hbar}H(\hat{p},\hat{x})}$ which not only reproduces the exact evolution of a wave function in the limit $\epsilon \to 0$, but also yields acceptable results when acting on position and momentum eigenstates $|x\rangle$ and $|p\rangle$ as in Eq. (2.31). We obtain such an approximation, which generalizes directly to the subsequent treatment of coherent state functional integrals, by considering a form of normal-ordered exponential.

For operators expressed in terms of $\hat{p}$ and $\hat{x}$, we will define an operator to be in normal form when all the $\hat{p}$'s appear to the left of all the $\hat{x}$'s, and the result of reordering an operator $O(\hat{p},\hat{x})$ into normal form will be denoted $:O(\hat{p},\hat{x}):$. For example, the Hamiltonian for a single particle in a potential

$$H_v(\hat{p},\hat{x}) = \frac{\hat{p}^2}{2m} + V(\hat{x}) \tag{2.32}$$

is in normal form and

$$:e^{-i\frac{\epsilon}{\hbar}H_v(\hat{p},\hat{x})}: \ = \sum_{n=0}^{\infty} (-i\frac{\epsilon}{\hbar})^n \sum_{k=0}^{n} \frac{1}{k!(n-k)!} \left(\frac{\hat{p}^2}{2m} \right)^k (V(\hat{x}))^{n-k} \ . \tag{2.33}$$

The Hamiltonian for a particle in a magnetic field described by a vector potential $A(x)$ may be rewritten in normal form as follows

$$\begin{aligned} H_A(\hat{p},\hat{x}) &= \frac{1}{2m}\left(\hat{\vec{p}} - \frac{e}{c}\vec{A}(\hat{x}) \right)^2 \\ &= \frac{1}{2m}\left(\hat{\vec{p}}^2 - \frac{e}{c} 2\hat{\vec{p}}\vec{A}(\hat{x}) - \frac{e}{c} i\vec{\nabla}\cdot\vec{A}(\hat{x}) + \left(\frac{e}{c} A(\hat{x}) \right)^2 \right) \ . \end{aligned} \tag{2.34}$$

For any $H(\hat{p},\hat{x})$ in normal form,

$$e^{-i\frac{\epsilon}{\hbar}H(\hat{p},\hat{x})} = :e^{-i\frac{\epsilon}{\hbar}H(\hat{p},\hat{x})}: - \left(\frac{\epsilon}{\hbar}\right)^2 \sum_{n=0}^{\infty} \frac{(-i\frac{\epsilon}{\hbar})^n}{(n+2)!} \left(H(\hat{p},\hat{x})^{n+2} - :[H(\hat{p},\hat{x})]^{n+2}: \right) \tag{2.35}$$

and for the special case Eq. (2.32), the leading correction is

$$-\frac{\epsilon^2}{2\hbar^2}\left[V, \frac{\hat{p}^2}{2m} \right] = -\frac{\epsilon^2}{4m\hbar^2}(V'' + 2iV'\hat{p}) \ . \tag{2.36}$$

Thus, if the infinitesimal evolution operator is approximated by the normal-ordered evolution operator, the error is of order ϵ^2 times an operator which may be expressed in terms of multiple commutators of the operators comprising the Hamiltonan. When acting upon a normalizable, differentiable wave function $\psi(x)$, the error term is ϵ^2 times a finite number, so that in the limit $\epsilon \to 0$, we are assured that $:e^{-i\frac{\epsilon}{\hbar}H(\hat{p},\hat{x})}:$ yields the correct evolution of the wave function. Furthermore, in contrast to other approximations which are valid to first order in ϵ, the normal-ordered evolution operator may be used in the integral in Eq. (2.31).

$$\begin{aligned} \langle x_n | :e^{-i\frac{\epsilon}{\hbar}H(\hat{p},\hat{x})}: | x_{n-1} \rangle &= \int d^3 p_n \langle x_n | p_n \rangle \langle p_n | :e^{-i\frac{\epsilon}{\hbar}H(\hat{p},\hat{x})}: | x_{n-1} \rangle \\ &= \int \frac{d^3 p_n}{(2\pi\hbar)^3} e^{ip_n(x_n - x_{n-1})} e^{-i\frac{\epsilon}{\hbar}H(p_n, x_{n-1})} \ . \end{aligned} \tag{2.37}$$

For the case of a particle in a potential, Eq. (2.32), this integral over p is a Gaussian integral yielding

$$\begin{aligned} \langle x_n | e^{-i\frac{\epsilon}{\hbar}\left(\frac{\hat{p}^2}{2m} + V(\hat{x})\right)} | x_{n-1} \rangle &= \langle x_n | :e^{-i\frac{\epsilon}{\hbar}\left(\frac{\hat{p}^2}{2m} + V(\hat{x})\right)}: | x_{n-1} \rangle + O(\epsilon^2) \\ &= \int \frac{d^3 p}{(2\pi\hbar)^3} e^{i\frac{p}{\hbar}(x_n - x_{n-1}) - i\frac{\epsilon}{\hbar}\frac{p^2}{2m} - i\frac{\epsilon}{\hbar}V(x_{n-1})} + O(\epsilon^2) \\ &= \left(\frac{m}{2\pi i\epsilon\hbar} \right)^{\frac{3}{2}} e^{\frac{i}{\hbar}\left(\frac{m}{2\epsilon}(x_n - x_{n-1})^2 - \epsilon V(x_{n-1})\right)} + O(\epsilon^2) \ . \end{aligned} \tag{2.38}$$

At this point, approximating the infinitesimal evolution operator by $:e^{-i\frac{\epsilon}{\hbar}\left(\frac{\hat{p}^2}{2m} + V(\hat{x})\right)}:$ instead of $1 - i\frac{\epsilon}{\hbar}\left(\frac{\hat{p}^2}{2m} + V(\hat{x})\right)$ or some other expression valid to order ϵ may well appear artificial. The essential issue is to obtain an approximation

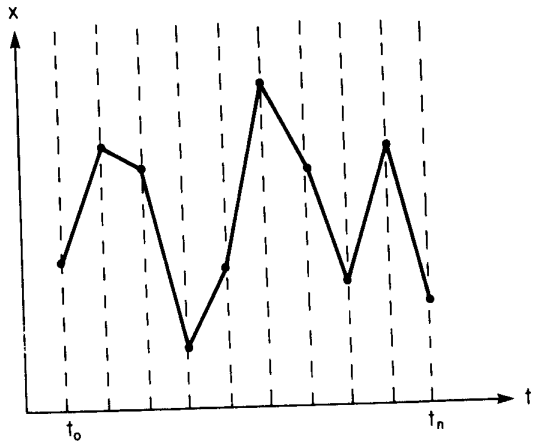

Fig. 2.3 A typical trajectory contributing to a path integral.

yielding convergent momentum integrals both in the present case of real time and in subsequent expressions continued to imaginary time. Whereas individual terms in the Taylor series expansion yield powers of p which diverge, since p^2 is bounded from below, both $e^{-\frac{i}{\hbar}\frac{p^2}{2m}}$ and $e^{-\epsilon\frac{1}{\hbar}\frac{p^2}{2m}}$ are bounded. Mathematically precise derivations of successive levels of generality are provided by Simon (1979), Trotter (1959), and Kato (1978).

Although it is crucial to use a form in which p^2 has been exponentiated, there still remains some arbitrariness in the approximation Eq. (2.37). As shown in Problem 2.4, one may replace $V(x_{n-1})$ by $V(x_n)$ or $\frac{1}{2}(V(x_{n-1})+V(x_n))$ and in applications such as in Chapter 8 where ϵ remains finite, this freedom may be exploited to improve the approximation.

The problems arising when the Hamiltonian contains terms in which $\hat{p}$ and $\hat{x}$ are combined are exhibited in Problem 2.5 for a particle in a magnetic field. The ultimate justification for any expression such as Eq. (2.38) used to approximate $\langle x_n|e^{-\frac{i}{\hbar}\left(\frac{\hat{p}^2}{2m}+V(\hat{x})\right)}|x_{n-1}\rangle$ is that it reproduces the correct evolution of the wave function, and this may be verified straightforwardly (see Problems 2.4 and 2.5).

Using Eq. (2.38) and the notation of Eq. (2.29), the matrix element of the evolution operator Eq. (2.30) may be written

$$U(x_f t_f, x_i t_i) = \lim_{M\to\infty}\int\prod_{k=1}^{M-1} dx_k \left(\frac{m}{2\pi i\epsilon\hbar}\right)^{\frac{1}{2}M} e^{\frac{i}{\hbar}\epsilon\sum_{k=1}^{M}\left(\frac{m}{2}\left(\frac{x_k-x_{k-1}}{\epsilon}\right)^2-V(x_{k-1})\right)} . \tag{2.39}$$

The set of points $\{x_o, x_1, \ldots x_M\}$ defines a trajectory as sketched in Fig. 2.3. For notational convenience, in the limit $M\to\infty$ we will often denote this trajectory by $x(t)$ with starting point $x(t_i)=x_i$ and endpoint $x(t_f)=x_f$, but it is crucial to note that this notation does not imply continuity or differentiability. Rather, the trajectory should always be thought of as a set of M points $x(t_k)$ indexed by the discrete times

t_k. In the same spirit, it is convenient to represent $\frac{x_k-x_{k-1}}{\epsilon}$ by the symbol $\frac{dx}{dt}$. Again, no differentiability is implied and the precise definition of $\frac{dx}{dt}$ is given by the finite-difference expression. With this notation, the Riemann sums in the exponent may be indicated symbolically

$$\epsilon\sum_{k=1}^{M}\frac{m}{2}\left(\frac{x_k-x_{k-1}}{\epsilon}\right)^2 \to \int_{t_i}^{t_f} dt\,\frac{m}{2}\left[\frac{dx}{dt}\right]^2 \tag{2.40a}$$

and

$$\epsilon\sum_{k=1}^{M} V(x_{k-1}) \to \int_{t_i}^{t_f} dt\, V(x(t)) \ . \tag{2.40b}$$

The Feynman path integral, which is defined as the limit of Eq. (2.39) as $M\to\infty$, is denoted

$$U(x_f t_f, x_i t_i) = \int_{(x_i,t_i)}^{(x_f,t_f)} \mathcal{D}[x(t)]e^{\frac{i}{\hbar}\int_{t_i}^{t_f} dt\left(\frac{m}{2}\left(\frac{dx}{dt}\right)^2-V(x(t))\right)} = \int_{(x_i,t_i)}^{(x_f,t_f)} \mathcal{D}[x(t)]e^{\frac{i}{\hbar}S[x(t)]} \tag{2.41}$$

where

$$\int_{(x_i,t_i)}^{(x_f,t_f)} \mathcal{D}[x(t)] = \lim_{M\to\infty}\int\prod_{k=1}^{M-1} dx_k\left(\frac{m}{2\pi i\epsilon\hbar}\right)^{\frac{1}{2}M} \tag{2.42}$$

represents a sum over all trajectories starting at position x_i at time t_i and ending at position x_f at time t_f, the action $S[x(t)]$ is

$$S[x(t)] = \int_{t_i}^{t_f} dt L[x(t)] \tag{2.43}$$

and the Lagrangian $L[x(t)]$ is

$$L[x(t)] = \frac{1}{2}m\left(\frac{dx}{dt}\right)^2 - V(x(t)) \ . \tag{2.44}$$

The matrix element of the evolution operator between states $|x_i\rangle$ and $|x_f\rangle$ is thus the sum over all trajectories beginning at x_i at time t_i and ending at x_f at time t_f of the exponential $\frac{i}{\hbar}$ times the action along the trajectory.

Several remarks concerning the Feynman path integral, Eq. (2.41) are germane at this point. Because the path integral is an exact representation of the evolution operator, it may be used as the starting point for the formulation of quantum mechanics (see Feynman and Hibbs (1965)). The superposition principle, which may be written at any time t in the form

$$U(x_f t_f, x_i t_i) = \int dx U(x_f t_f, xt)U(xt, x_i t_i) \tag{2.45}$$

is expressed in terms of path integrals as

$$\int_{(x_i t_i)}^{(x_f t_f)} \mathcal{D}[x(t)] e^{\frac{i}{\hbar}\int_{t_i}^{t_f} dt' L[x(t')]} = \int dx \int_{(xt)}^{(x_f t_f)} \mathcal{D}[x(t)] e^{\frac{i}{\hbar}\int_{t}^{t_f} dt' L[x(t')]} \times \int_{(x_i t_i)}^{(x,t)} \mathcal{D}[x(t)] e^{\frac{i}{\hbar}\int_{t_i}^{t} dt' L[x(t')]} \tag{2.46}$$

and quantum mechanical interference arises directly from the sums over trajectories. A natural approximation to the path integral, Eq. (2.41) in the limit as $\hbar \to 0$ is the stationary-phase approximation. As will be shown in detail in Section (2.5), the dominant contribution to the transition amplitude in this limit comes from trajectories surrounding the classical trajectory joining x_i to x_f. Finally, since the measure in Eq. (2.42) is still ill-defined when ϵ goes to zero, it is useful to note that the functional integral may be normalized by solutions of an analytically solvable reference problem. For example, one may require that when the potential V is set to zero, the transition amplitude is

$$\begin{aligned} U_0(x_f t_f, x_i t_i) &= \langle x_f | e^{\frac{i}{\hbar}\frac{\hat{p}^2}{2m}(t_f - t_i)} | x_i \rangle \\ &= \left[\frac{m}{2\pi i\hbar(t_f - t_i)}\right]^{\frac{3}{2}} e^{i\frac{m}{2\hbar}\frac{(x_f - x_i)^2}{t_f - t_i}} . \end{aligned} \tag{2.47}$$

The functional integral in Eq. (2.41) is called the Lagrangian form and requires that the Hamiltonian have quadratic momentum dependence as in Eq. (2.32). The Hamiltonian form of the functional integral is obtained by substituting Eq. (2.37) in Eq. (2.30) without performing the p integration, in which case the matrix element of the evolution operator becomes

$$\begin{aligned} U(x_f t_f, x_i t_i) = \lim_{M\to\infty} \int \prod_{k=1}^{M-1} dx_k \prod_{k=1}^{M} \frac{dp_k}{(2\pi\hbar)^3} e^{\frac{i}{\hbar}\sum_{k=1}^{M}[p_k(x_k - x_{k-1}) - \epsilon\frac{p_k^2}{2m} - \epsilon V(x_{k-1})]} \\ \to \int_{(x_i t_i)}^{(x_f t_f)} \mathcal{D}[x(t)]\mathcal{D}[p(t)] e^{\frac{i}{\hbar}\int_{t_i}^{t_f} dt[p(t)\frac{\partial}{\partial t}x(t) - H(p(t),x(t))]} . \end{aligned} \tag{2.48}$$

The trajectories $x(t)$ obey the same boundary conditions as in the Lagrangian form and the trajectories $p(t)$ have no boundary conditions. The Hamiltonian form of this functional integral is *a priori* more general than the Lagrangian form, but requires care in the ordering of the non-commuting operators $\hat{x}$ and $\hat{p}$ when $\mathcal{H}$ contains mixed terms in $\hat{x}$ and $\hat{p}$ (see Problem 2.5).

At this point, it is useful to note that path integrals automatically represent time-ordered products. Let $\mathcal{O}_1(\hat{x}, t_1)$ and $\mathcal{O}_2(\hat{x}, t_2)$ be operators acting at times t_1 and t_2 with $t_1 \geq t_2$ and let t_m denote the discrete time in Eq. (2.30) closest to t_1 and t_n denote the discrete time closest to t_2. Then

$$\begin{aligned} &\langle x_f | T\mathcal{O}_1(\hat{x}, t_1)\mathcal{O}_2(\hat{x}, t_2) e^{-\frac{i}{\hbar}\int_{t_i}^{t_f}\hat{H}(t)dt} | x_i \rangle \\ &= \langle x_f | T e^{-\frac{i}{\hbar}\int_{t_1}^{t_f}\hat{H}(t)dt} \mathcal{O}(\hat{x}, t_1) T e^{-\frac{i}{\hbar}\int_{t_2}^{t_1}\hat{H}(t)dt} \mathcal{O}(\hat{x}, t_2) T e^{-\frac{i}{\hbar}\int_{t_i}^{t_2}\hat{H}(t)dt} | x_i \rangle \\ &= \lim \int \prod_{k=1}^{M-1} dx_k \langle x_f | e^{-i\frac{\epsilon}{\hbar}H} \ldots | x_m \rangle \langle x_m | \mathcal{O}_1(\hat{x}) e^{-i\frac{\epsilon}{\hbar}H} | x_{m-1} \rangle \langle x_{m-1} | \ldots \\ &\quad \times e^{-i\frac{\epsilon}{\hbar}H} | x_n \rangle \langle x_n | \mathcal{O}_2(\hat{x}) e^{-i\frac{\epsilon}{\hbar}H} | x_{n-1} \rangle \langle x_{n-1} | \ldots e^{-i\frac{\epsilon}{\hbar}H} | x_i \rangle \\ &= \int_{(x_i t_i)}^{(x_f t_f)} \mathcal{D}[x(t)] \mathcal{O}_1(x(t_1)) \mathcal{O}_2(x(t_2)) e^{\frac{i}{\hbar}\int_{t_i}^{t_f} dt L[x(t)]} \\ &= \int_{(x_i t_i)}^{(x_f t_f)} \mathcal{D}[x(t)]\mathcal{D}[p(t)] \mathcal{O}_1(x(t_1)) \mathcal{O}(x(t_2)) e^{\frac{i}{\hbar}\int_{t_i}^{t_f} dt(p(t)\dot{x}(t) - H[p(t),x(t)])} . \end{aligned} \tag{2.49}$$

Thus, although there is no explicit indication in the notation that operators have been time-ordered, in order for the operators $\mathcal{O}_1(\hat{x}, t_1)$, $\mathcal{O}_2(\hat{x}, t_2)$, and $\hat{H}(t)$ to be replaced by the c-numbers $\mathcal{O}_1(x(t_1))$, $\mathcal{O}_2(x(t_2))$, and $H[p(t), x(t)]$, it is implicit in the construction of the functional integral that each operator had to act on the complete set of states introduced at the corresponding discrete time. Operators depending upon the momentum $\hat{p}$ are treated in the same way by letting them act on the complete set of momentum states introduced at the corresponding time. The fact that functional integrals necessarily yield time-ordered products is the reason for the assertion in Section 2.1 that time-ordered products are the quantities which arise naturally in the formalism and that physical response functions should ultimately be evaluated in terms of them. From the definition of the time-ordered exponential, Eq. (2.9), and the path integral, it is evident that both quantities deal with the non-commutativity of operators in quantum mechanics in the same way. In both cases the time interval is divided into sufficiently small subintervals that the commutator terms $\frac{\epsilon^2}{2}[\frac{p^2}{2m}, V]$ become negligible. There is no reason why the continuous parameter must necessarily be the physical time, and we will see that it is also useful to use temperature (or imaginary time) as the formal parameter for developing path integrals.

IMAGINARY-TIME PATH INTEGRAL AND THE PARTITION FUNCTION

The partition function for a single particle may be written

$$\begin{aligned} Z &= \mathrm{Tr}\, e^{-\beta\hat{H}} \\ &= \int dx \langle x | e^{-\beta\hat{H}} | x \rangle \end{aligned} \tag{2.50}$$

and may be thought of as a sum over diagonal matrix elements of the imaginary time evolution operator

$$U(x_f\tau_f, x_i\tau_i) = \langle x_f|e^{-(\tau_f-\tau_i)\frac{\hat{H}}{\hbar}}|x_i\rangle \tag{2.51}$$

evaluated for the interval $\tau_f - \tau_i = \beta\hbar$. Note that for the one-particle problem, we work in the canonical ensemble and there is no chemical potential. Given the observation that the essence of a path integral or time-ordered exponential is the subdivision of the interval into sufficiently small intervals that commutators of the quantum operator appearing in H may be neglected, all the steps in the derivation of the real-time path integral may be repeated for the case of imaginary time. For the Hamiltonian, Eq. (2.32), we obtain

$$\begin{aligned}
U(x_f t_f, x_i t_i) &= \lim_{M\to\infty}\int\prod_{k=1}^{M-1} d^3x_k \prod_{k=1}^{M}\langle x_k|e^{-\frac{\epsilon}{\hbar}H(\hat{p},\hat{x})}|x_{k-1}\rangle \\
&= \lim_{M\to\infty}\int\prod_{k=1}^{M-1} d^3x_k \prod_{k=1}^{M} d^3p_k\langle x_k|p_k\rangle\langle p_k|:e^{-\frac{\epsilon}{\hbar}H(\hat{p},\hat{x})}: + O\epsilon^2|x_{k-1}\rangle \\
&= \lim_{M\to\infty}\int\prod_{k=1}^{M-1} d^3x_k \prod_{k=1}^{M}\frac{d^3p_k}{(2\pi\hbar)^3} e^{\sum_{k=1}^{M}\left[\frac{ip_k}{\hbar}(x_k-x_{k-1})-\frac{\epsilon}{\hbar}\left(\frac{p_k^2}{2m}+V(x_{k-1})\right)\right]} \\
&= \lim_{M\to\infty}\int\prod_{k=1}^{M-1} d^3x_k \left(\frac{m}{2\pi\epsilon\hbar}\right)^{\frac{3M}{2}} e^{-\frac{\epsilon}{\hbar}\sum_{k=1}^{M}\left[\frac{m}{2}\frac{(x_k-x_{k-1})^2}{\epsilon^2}+V(x_{k-1})\right]} \\
&= \int_{(x_i,\tau_i)}^{(x_f,\tau_f)}\mathcal{D}[x(\tau)]e^{-\frac{1}{\hbar}\int_{\tau_i}^{\tau_f}d\tau\left(\frac{m}{2}\left(\frac{dx(\tau)}{d\tau}\right)^2+V(x(\tau))\right)} \\
&= \int_{(x_i,\tau_i)}^{(x_f,\tau_f)}\mathcal{D}[x(\tau)]e^{-\frac{1}{\hbar}\int_{\tau_i}^{\tau_f}dtH[x(\tau)]}
\end{aligned} \tag{2.52}$$

where $\epsilon = \frac{1}{M}(\tau_f - \tau_i)$. Thus, the imaginary-time path integral is a sum over trajectories starting at (x_i, τ_i) and ending at (x_f, τ_f) of the exponential of a modified action in which a change in sign of the kinetic term yields the Hamiltonian instead of the Lagrangian.

An alternative derivation, which shows explicitly how the Lagrangian in the real-time case is transformed into the Hamiltonian in the imaginary time case, is to preform an analytic continuation of Eq. (2.41) to imaginary time. This continuation, known as a Wick rotation because it may be viewed as a rotation of the integration contour in the complex t-plane, is effected by the variable transformation

$$t = -i\tau \ . \tag{2.53a}$$

Thus,

$$\frac{dx}{d\tau} = \frac{dt}{d\tau}\frac{dx}{dt} = -i\frac{dx}{dt} \tag{2.53b}$$

and the action, which is called the Euclidean action, becomes

$$\frac{i}{\hbar}\int_{t_1}^{t_2}dt\left[\frac{m}{2}\left(\frac{dx}{dt}\right)^2 - V(x(t))\right] = -\frac{1}{\hbar}\int_{\tau_1}^{\tau_2}d\tau\left[\frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 + V(x(\tau))\right] \ . \tag{2.53c}$$

The kinetic energy thus changes signs because each time derivative acquires a factor of i. The same sign reversal arises in the classical equations of motion in imaginary time, and the interpretation of a particle moving in an inverted potential will subsequently provide a picturesque way to visualize the stationary solutions to path integrals in classically forbidden regimes.

For the imaginary-time path integral, the measure appearing in Eq. (2.52) is equivalent to the Wiener measure defined in the study of continuous stochastic processes (Wiener, (1924,1932)) and the functional integral can be given a rigorous mathematical definition. This path integral will provide the foundation of the stochastic method presented in Chapter 8, and the nature of the trajectories which contribute to it will be studied more thoroughly in that context.

Using Eqs. (2.50) – (2.52), the partition function may be expressed

$$\begin{aligned}
Z &= \int dx \int_{x(0)=x}^{x(\beta\hbar)=x}\mathcal{D}[x(\tau)]e^{-\frac{1}{\hbar}\int_0^{\beta\hbar}d\tau\left(\frac{m}{2}\left(\frac{dx(\tau)}{d\tau}\right)^2+V(x(\tau))\right)} \\
&\equiv \int_{x(\beta\hbar)=x(0)}\mathcal{D}[x(\tau)]e^{-\frac{1}{\hbar}\int_0^{\beta\hbar}d\tau\left(\frac{m}{2}\left(\frac{dx(\tau)}{d\tau}\right)^2+V(x(\tau))\right)} \ .
\end{aligned} \tag{2.54}$$

The partition function is thus a sum over all periodic trajectories of period $\beta\hbar$ and the shorthand notation in the last line emphasizes the fact that the integral over x_m at the endpoint of the interval is equivalent to the integral over each of the internal x_k's within the interval. For notational clarity, except when we are specifically concerned with the classical limit in which $\hbar \to 0$, it will be convenient to use units in which $\hbar = 1$.

Finally, the Feynman path integral in real or imaginary time may be straightforwardly extended to many-particle systems. For example, using the symmetrized or antisymmetrized states defined in Eq. (1.38) where we used $\varsigma = \pm 1$ for Bosons or Fermions, the partition function for an N-particle system may be written

$$\begin{aligned}
Z &= \frac{1}{N!}\int\prod_{i=1}^{N}dx_i\,\{x_1\ldots x_n|e^{-\beta H}|x_1\ldots x_n\} \\
&= \frac{1}{N!}\sum_p \varsigma^p\int\prod_{i=1}^{N}dx_i(x_{p1}\ldots x_{pN}|e^{-\beta H}|x_1\ldots x_n) \ .
\end{aligned} \tag{2.55}$$

As in the case of a simple variable, the time interval β may be divided into infinitesimal steps. However, now we have the additional choice of inserting at each step the

closure relation Eq. (1.30) with product states or Eq. (1.40) using symmetrized or antisymmetrized states. Either choice yields exact evolution and the symmetry or antisymmetry of the final states in the trace suffices to impose the proper statistics. The use of product states yields the simplest formal result completely analogous to Eq. (2.52), and for the case of a Hamiltonian of the form

$$H = \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m} + \frac{1}{2}\sum_{i\neq j} v(\hat{x}_i - \hat{x}_j) \tag{2.56}$$

the partition function may be written

$$Z = \frac{1}{N!}\sum_P \zeta^P \int_{\substack{x_1(\beta)=x_{P1}(0)\\ x_N(\beta)=x_{PN}(0)}} \mathcal{D}[x_1(\tau)]\ldots\mathcal{D}[x_N(\tau)] \times e^{-\int_0^\beta d\tau\left[\sum_{i=1}^N \frac{m}{2}\left(\frac{dx_i(\tau)}{d(\tau)}\right)^2 + \frac{1}{2}\sum_{i\neq j} v(x_i(\tau)-x_j(\tau))\right]} . \tag{2.57}$$

In the case of stochastic evolution of path integrals for Fermions, the alternative choice of using antisymmetrized states at intermediate steps will prove advantageous in certain applications, as discussed in Chapter 8.

COHERENT STATE FUNCTIONAL INTEGRAL

For a general many-particle Hamiltonian expressed in second quantized form, a functional integral representation for the many-body evolution operator may be obtained using the coherent states $|\phi\rangle$, Eq. (1.118) and (1.160) instead of the position and momentum eigenstates used for the Feynman path integral. Recall that the relations for Fermions and Bosons have the identical form tabulated in Table 1.1 at the end of Chapter 1 where the integration variables are understood to be complex variables for Bosons and Grassman variables for Fermions. We will evaluate the matrix element of the evolution operator between an initial coherent state $|\phi_i\rangle$ having components $\phi_{\alpha,i}$ and a final state $\langle\phi_f|$ with components $\phi^*_{\alpha,f}$. As before, the integral $[t_i, t_f]$ is broken into M times steps of size $\epsilon = \frac{t_f - t_i}{M}$, a closure relation in the notation of Table 1.1

$$1 = \frac{1}{\mathcal{N}}\prod_\alpha d\phi^*_{\alpha,k} d\phi_{\alpha,k} e^{-\sum_\alpha \phi^*_{\alpha,k}\phi_{\alpha,k}} |\phi_{\alpha,k}\rangle\langle\phi_{\alpha,k}|$$

is inserted at the k^{th} time step, and we use the notation at the end points:

$$\begin{aligned} \phi_{\alpha,0} &\equiv \phi_{\alpha,i} \\ \phi^*_{\alpha,M} &\equiv \phi^*_{\alpha,f} \end{aligned} . \tag{2.58}$$

For second quantized operators, the appropriate form of normal ordering is that defined in Section (1.4) with all creation operators to the left of annihilation operators, and we will assume that $H(a^\dagger_\alpha, a_\alpha)$ is written in normal form. As in the path integral case,

$$e^{\epsilon H(a^\dagger a)} = :e^{\epsilon H(a^\dagger a)}: + \mathcal{O}(\epsilon^2) \tag{2.59}$$

where the term of order ϵ^2 is ϵ^2 times an operator which is finite when acting on a normalized, differential wave function $\psi(\phi^*_\alpha)$. Thus, using Eqs. (1.137) or (1.177) to evaluate coherent state matrix elements of the normal ordered exponentials, the matrix element of the evolution operator may be written

$$\begin{aligned} \mathcal{U}(\phi^*_{\alpha,f} t_f; \phi_{\alpha,i} t_i) &= \lim_{M\to\infty} \langle\phi_f| e^{-\frac{i}{\hbar}H(t_f - t_i)} |\phi_i\rangle \\ &= \lim_{M\to\infty} \int \prod_{k=1}^{M-1}\prod_\alpha \frac{1}{\mathcal{N}} d\phi^*_{\alpha,k} d\phi_{\alpha,k} e^{-\sum_{k=1}^{M-1}\sum_\alpha \phi^*_{\alpha,k}\phi_{\alpha,k}} \\ &\quad \times \prod_{k=1}^{M} \langle\phi_k| :e^{-\frac{i\epsilon}{\hbar}H(a^\dagger_\alpha, a_\alpha)}: + \mathcal{O}(\epsilon^2) |\phi_{k-1}\rangle \\ &= \lim_{M\to\infty} \int \prod_{k=1}^{M-1}\prod_\alpha \frac{1}{\mathcal{N}} d\phi^*_{\alpha,k} d\phi_{\alpha,k} e^{-\sum_{k=1}^{M-1}\sum_\alpha \phi^*_{\alpha,k}\phi_{\alpha,k}} \\ &\quad \times e^{\sum_{k=1}^{M}\left(\sum_\alpha \phi^*_{\alpha,k}\phi_{\alpha,k-1} - \frac{i\epsilon}{\hbar}H(\phi^*_{\alpha,k}\phi_{\alpha,k-1})\right)} . \end{aligned} \tag{2.60}$$

Note that in the case of Fermions, since there is no metric in the Grassman algebra, all the integrals indicated in Eq. (2.60) are finite. For Bosons, the argument is analogous to that for the path integral case. In real time $e^{-\frac{i\epsilon}{\hbar}H}$ is oscillatory and the factor $e^{\phi^*_{\alpha,k}\phi_{\alpha,k}}$ arising from the measure produces convergence. In imaginary time we again rely upon the physical fact that the Hamiltonian is bounded from below, which implies that $H(\phi^*_{\alpha,k}, \phi_{\alpha,k-1}) \equiv \frac{\langle\phi_k|H|\phi_{k-1}\rangle}{\langle\phi_k|\phi_{k-1}\rangle}$ is also bounded from below. Hence $e^{-\frac{\epsilon}{\hbar}H(\phi^*_{\alpha,k},\phi_{\alpha,k-1})}$ is bounded and the Gaussian factor from the measure again ensures convergence.

As in the case of the path integral, it is convenient to introduce a trajectory $\phi_\alpha(t)$ to represent the set $\{\phi_{\alpha,1}\phi_{\alpha,2}\ldots\phi_{\alpha,M}\}$ and to introduce the notation

$$\phi^*_{\alpha,k}\frac{(\phi_{\alpha,k} - \phi_{\alpha,k-1})}{\epsilon} \equiv \phi^*_\alpha(t)\frac{\partial}{\partial t}\phi_\alpha(t) \tag{2.61a}$$

and

$$H(\phi^*_{\alpha,k}; \phi_{\alpha,k-1}) \equiv H(\phi^*_\alpha(t), \phi_\alpha(t)) \tag{2.61b}$$

in which case the exponent in Eq. (2.50) may be rewritten symbolically

$$\begin{aligned} &\sum_\alpha \phi^*_{\alpha,M}\phi_{\alpha,M-1} - i\frac{\epsilon}{\hbar}H(\phi^*_{\alpha,M}; \phi_{\alpha,M-1}) \\ &\quad + i\epsilon\sum_{k=1}^{M-1}\left[i\sum_\alpha \phi^*_{\alpha,k}\left(\frac{\phi_{\alpha,k} - \phi_{\alpha,k-1}}{\epsilon}\right) - \frac{1}{\hbar}H(\phi^*_{\alpha,k}; \phi_{\alpha,k-1})\right] \\ &\quad = \sum_\alpha \phi^*_\alpha(t_f)\phi_\alpha(t_f) + \frac{i}{\hbar}\int_{t_i}^{t_f} dt\left[\sum_\alpha i\hbar\phi^*_\alpha(t)\frac{\partial\phi_\alpha(t)}{\partial t} - H(\phi^*_\alpha(t), \phi_\alpha(t))\right] \\ &\quad = \sum_\alpha \phi^*_\alpha(t_f)\phi_\alpha(t_f) + \frac{i}{\hbar}\int_{t_i}^{t_f} dt L(\phi^*_\alpha(t), \phi_\alpha(t)) \end{aligned} \tag{2.61c}$$

where the Schrödinger Lagrangian operator is $i\hbar\frac{\partial}{\partial t} - H$. As in the Feynman path integral, the trajectory and derivative notation is purely symbolic, and for any case in which ambiguity may arise, the correct physical quantity is calculated by performing the integral over the discrete action in Eq. (2.61c) and then taking the limit $M \to \infty$. With this notation,

$$U(\phi^*_{\alpha,f}, t_f; \phi_{\alpha,i} t_i) = \int_{\phi_\alpha(t_i)=\phi_{\alpha,i}}^{\phi^*_\alpha(t_f)=\phi^*_{\alpha,f}} \mathcal{D}[\phi^*_\alpha(t)\phi_\alpha(t)] e^{\sum_\alpha \phi^*_\alpha(t_f)\phi_\alpha(t_f)} \times e^{\frac{i}{\hbar}\int_{t_i}^{t_f} dt \left[\sum_\alpha i\hbar\phi^*_\alpha(t)\frac{\partial\phi_\alpha(t)}{\partial t} - H(\phi^*_\alpha(t),\phi_\alpha(t))\right]} \tag{2.62a}$$

where

$$\int_{\phi_\alpha(t_i)}^{\phi^*_\alpha(t_f)} \mathcal{D}[\phi^*_\alpha(t)\phi_\alpha(t)] = \lim_{M\to\infty} \int \prod_{k=1}^{M-1} \prod_\alpha \frac{1}{\mathcal{N}} d\phi^*_{\alpha,k} d\phi_{\alpha,k} \ . \tag{2.62b}$$

Note in the discrete expression, that the boundary conditions specified $\phi_{\alpha,0}$ and $\phi^*_{\alpha,M}$, that there were no variables $\phi^*_{\alpha,0}$ or $\phi_{\alpha,M}$, and that all the internal conjugate variables $\phi^*_{\alpha,k}$ and $\phi_{\alpha,k}$ for $k = 1, M-1$ are integrated. In the trajectory notation $\phi^*_\alpha(t)$ and $\phi_\alpha(t)$ are associated with variables displaced by one time step, $\phi^*_{\alpha,k}$ and $\phi_{\alpha,k-1}$, respectively, so that $\phi^*_\alpha(t_f)$ and $\phi_\alpha(t_i)$ are specified by the boundary conditions but $\phi_\alpha(t_f)$ and $\phi^*_\alpha(t_f)$ correspond to internal variables of integration not subject to boundary conditions. The boundary term $\phi^*_{\alpha,M}\phi_{\alpha,M-1}$ appearing in the exponent, Eq. (2.61c) represents a term left over at the end of the path from our grouping of terms in defining the derivative Eq. (2.61a). Had we chosen the alternative convention $\frac{1}{\epsilon}(-\phi^*_{\alpha,k+1} + \phi^*_{\alpha,k})\phi_{\alpha,k} = \left(-\frac{\partial}{\partial t}\phi^*_\alpha(t)\right)\phi(t)$,the remaining boundary term would have been $\phi^*_1\phi_0$. Both results correspond to the same fundamental discrete expression and are thus equivalent. If a symmetric formal expression is desired, one may use the average of the two.

One significant difference between the coherent state functional integral, Eq. (2.62) and the Feynman path integral is the dependence upon $\hbar$. In the Feynman case, $\frac{1}{\hbar}$ appears as a constant multiplying the entire exponent, so that the stationary-phase expansion immediately yields the classical limit. In the present case, the action contains $\hbar$ within the Lagrangian as well as a multiplicative factor, so that the stationary-phase method yields a result quite distinct from the classical limit.

THE PARTITION FUNCTION FOR MANY-PARTICLE SYSTEMS

As in Eq. (2.57), the partition function for a many-particle system may be expressed as the trace of an imaginary-time evolution operator. Using Eqs. (1.128) or (1.173) for the trace with Boson or Fermion coherent states and units such that $\hbar = 1$, the partition function may be written

$$\begin{aligned} Z &= \mathrm{Tr}\, e^{-\beta(\hat{H}-\mu\hat{N})} \\ &= \int \prod_\alpha d\phi^*_\alpha d\phi_\alpha e^{-\sum_\alpha \phi^*_\alpha\phi_\alpha} \langle \varsigma\phi | e^{-\beta(\hat{H}-\mu\hat{N})} | \phi\rangle \ . \end{aligned} \tag{2.63}$$

When the continuation of Eq. (2.50) to imaginary time is substituted in this expression, the trace imposes the periodic or antiperiodic boundary conditions

$$\begin{aligned} \phi_{\alpha,0} &= \phi_\alpha \\ \phi^*_{\alpha,M} &= \varsigma\phi^*_\alpha \ . \end{aligned} \tag{2.64}$$

The equivalence of the interior and exterior coherent state integrals is emphasized by relabelling $\phi_\alpha \equiv \varsigma\phi_{\alpha,M}$ and the resulting partition function is

$$Z = \lim_{M\to\infty} \int \prod_{k=1}^{M} \prod_\alpha \frac{1}{\mathcal{N}} d\phi^*_{\alpha,k} d\phi_{\alpha,k} e^{-S(\phi^*,\phi)} \tag{2.65a}$$

where

$$\begin{aligned} S(\phi^*,\phi) = \epsilon \sum_{k=2}^{M} \left[\sum_\alpha \phi^*_{\alpha k}\left\{\frac{(\phi_{\alpha,k}-\phi_{\alpha,k-1})}{\epsilon} - \mu\phi_{\alpha,k-1}\right\} + H(\phi^*_{\alpha,k},\phi_{\alpha,k-1})\right] \\ + \epsilon\left[\sum_\alpha \phi^*_{\alpha 1}\left\{\frac{\phi_{\alpha,1}-\varsigma\phi_{\alpha,M}}{\epsilon} - \mu\varsigma\phi_{\alpha,M}\right\} + H(\phi^*_{\alpha 1},\varsigma\phi_{\alpha,M})\right] \ . \end{aligned} \tag{2.65b}$$

Using the trajectory notation, this may be rewritten

$$Z = \int_{\phi_\alpha(\beta)=\varsigma\phi_\alpha(0)} \mathcal{D}(\phi^*_\alpha(\tau)\phi_\alpha(\tau)) e^{-\int_0^\beta d\tau \left\{\sum_\alpha \phi^*_\alpha(\tau)(\frac{\partial}{\partial\tau}-\mu)\phi_\alpha(\tau) + H(\phi^*_\alpha(\tau),\phi_\alpha(\tau))\right\}} \tag{2.66}$$

with the usual understanding that the derivatives and integrals are defined in terms of the discrete expression, Eq. (2.62). Note that the integration is over complex variables satisfying periodic boundary conditions for Bosons and Grassman variables satisfying antiperiodic boundary conditions for Fermions.

In a formal sense, the problem has now been reduced to quadrature and we only need to develop techniques to evaluate the integral in Eq. (2.62). Our overall approach will be to group the one-body part of $H(\phi^*,\psi)$ together with the other quadratic terms in the exponent and to develop a perturbation series in which the exponential of the many-body part of $H(\phi^*,\phi)$ is expanded in a Taylor series. This will give rise to a series of integrals of the products of a Gaussian times polynomials which may be evaluated straightforwardly using the techniques developed in the next section.

The thermal Green's function, defined in Eq(2.22), has a simple form expressed in terms of a coherent state path integral. It is useful to give the creation and annihilation operators a formal τ label,$\{a^\dagger_\alpha(\tau), a_\alpha(\tau)\}$, denoting the time slice τ upon which they are defined. This purely formal τ label is introduced to allow the time-ordering operator to appropriately interlace operators with no explicit τ-dependence, and when the evolution operator is represented by a functional integral, the operators $\{a^\dagger_\alpha(\tau), a_\alpha(\tau)\}$ on the time slice τ will be replaced by the coherent state variables $\{\psi^*_\alpha(\tau), \psi_\alpha(\tau)\}$. To facilitate manipulation of the time-ordered product, it is convenient to write the thermal Green's

function, Eq. (2.22), as follows:

$$\begin{aligned}\mathcal{G}^{(n)}(\alpha_1\tau_1\ldots\alpha_n\tau_n|\alpha_{2n}\tau_{2n}\ldots\alpha_{n+1}\tau_{n+1}) \qquad (2.67a)\\ = \frac{1}{Z}\mathrm{Tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}T\,a^{(H)}_{\alpha_1}(\tau_1)\ldots a^{(H)}_{\alpha_n}(\tau_n)a^{(H)\,\dagger}_{\alpha_{n+1}}(\tau_{n+1})a^{(H)\,\dagger}_{\alpha_{2n}}(\tau_{2n})\right]\\ = \frac{1}{Z}\mathrm{Tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}\zeta^P\tilde{a}^{(H)}_{\alpha_{P1}}(\tau_{P1})\tilde{a}^{(H)}_{\alpha_{P2}}(\tau_{P2})\ldots\tilde{a}^{(H)}_{\alpha_{P2N}}(\tau_{P2N})\right]\end{aligned}$$

where the permutation P arranges the times in chronological order and $\tilde{a}_{\alpha_i}$ is an annihilation operator for $i \le n$ and a creation operator for $i > n$. Using the definition of the Heisenberg operator, Eq(2.23), and the fact that a functional integral corresponds to a time-ordered product,Eq(2.49), the Green's function may be written as follows:

$$\begin{aligned}\mathcal{G}^{(n)}(\alpha_1\tau_1\ldots\alpha_n\tau_n|\alpha_{2n}\tau_{2n}\ldots\alpha_{n+1}\tau_{n+1}) \qquad (2.67b)\\ = \frac{1}{Z}\zeta\mathrm{Tr}\Big[e^{-\beta(\hat{H}-\mu\hat{N})}e^{\tau_{P1}(\hat{H}-\mu\hat{N})}\tilde{a}_{\alpha_{P1}}e^{-\tau_{P1}(\hat{H}-\mu\hat{N})}\\ \times e^{\tau_{P2}(\hat{H}-\mu\hat{N})}\tilde{a}_{\alpha_{P2}}e^{-\tau_{P2}(\hat{H}-\mu\hat{N})}\ldots e^{\tau_{P2n}(\hat{H}-\mu\hat{N})}\tilde{a}_{\alpha_{P2n}}e^{-\tau_{P2n}(\hat{H}-\mu\hat{N})}\Big]\\ = \frac{1}{Z}\zeta^P\mathrm{Tr}\Big[e^{-\int_{\tau_{P1}}^{\beta}(\hat{H}-\mu\hat{N})}\tilde{a}_{\alpha_{P1}}e^{-\int_{\tau_{P2}}^{\tau_{P1}}(\hat{H}-\mu\hat{N})}\tilde{a}_{\alpha_{P2}}\ldots\tilde{a}_{\alpha_{P2n}}e^{-\int_{0}^{\tau_{P2n}}(\hat{H}-\mu\hat{N})}\Big]\\ = \frac{1}{Z}\mathrm{Tr}\Big[Te^{-\int_0^\beta(\hat{H}-\mu\hat{N})}a_{\alpha_1}(\tau_1)\ldots a_{\alpha_N}(\tau_N)a^\dagger_{\alpha_{N+1}}(\tau_{N+1})\ldots a^\dagger_{\alpha_{2n}}(\tau_{2n})\Big]\\ = \frac{1}{Z}\int\mathcal{D}[\phi^*_\alpha(\tau)\phi_\alpha(\tau)]\Big[e^{-\int_0^\beta d\tau\left[\sum_\alpha\phi^*_\alpha(\tau)(\frac{\partial}{\partial\tau}-\mu)\phi_\alpha(\tau)+H[\phi^*_\alpha(\tau),\phi_\alpha(\tau)]\right]}\\ \times\phi_{\alpha_1}(\tau_1)\ldots\phi_{\alpha_n}(\tau_n)\phi^*_{\alpha_{n+1}}(\tau_{n+1})\ldots\phi^*_{\alpha_{2n}}(\tau_{2n})\Big]\ .\end{aligned}$$

As preparation for the general case of a many-body Hamiltonian, it is useful to evaluate the partition function for a system of non-interacting particles described by a one-body Hamiltonian. For convenience, we choose a basis in which H_0 is diagonal:

$$H_0 = \sum_\alpha \epsilon_\alpha a^\dagger_\alpha a_\alpha\ . \qquad (2.68)$$

The discrete expression for the partition function, Eq. (2.65), may be written

$$\begin{aligned}Z_0 = \lim_{M\to\infty}\prod_\alpha\left[\prod_{k=1}^{n}\int\frac{1}{\mathcal{N}}d\phi^*_k d\phi_k e^{-\sum_{j,k=1}^{M}\phi^*_j S^{(\alpha)}_{jk}\phi_k}\right] \qquad (2.69)\\ = \lim_{M\to\infty}\prod_\alpha[\det S^{(\alpha)}]^{-\zeta}\end{aligned}$$

where, with the convention that the time index increases with increasing row and column index

$$S^{(\alpha)} = \begin{bmatrix} 1 & 0 & & \ldots & 0 & -\zeta a\\ -a & 1 & 0 & & & 0\\ 0 & -a & 1 & \ddots & & \vdots\\ & 0 & -a & \ddots & 0 & \\ \vdots & & 0 & \ddots & 1 & 0\\ 0 & & & \ldots & -a & 1\end{bmatrix} \qquad \phi = \begin{bmatrix}\phi_1\\ \phi_2\\ \\ \vdots\\ \\ \phi_M\end{bmatrix} \qquad (2.70a)$$

and where

$$a = 1 - \frac{\beta}{M}(\epsilon_\alpha - \mu)\ . \qquad (2.70b)$$

The determinant of $S^{(\alpha)}$ may be evaluated by expanding by minors along the first row

$$\begin{aligned}\lim_{M\to\infty}\det S^{(\alpha)} &= \lim_{M\to\infty}\left[1+(-1)^{M-1}\zeta(-a)^M\right]\\ &= \lim_{M\to\infty}\left[1-\zeta\left(1-\frac{\beta(\epsilon_\alpha-\mu)}{M}\right)^M\right] \qquad (2.71)\\ &= 1-\zeta e^{-\beta(\epsilon_\alpha-\mu)}\ .\end{aligned}$$

Substitution in Eq. (2.69) yields the familiar result for non-interacting particles

$$Z_0 = \prod_\alpha\left(1-\zeta e^{-\beta(\epsilon_\alpha-\mu)}\right)^{-\zeta}\ . \qquad (2.72)$$

Note that $\frac{1}{\epsilon}S$ arising from the definition of the functional integral corresponds to a specific discrete approximation to the continuum operator $\frac{\partial}{\partial\tau}+\epsilon_\alpha-\mu$ with periodic or antiperiodic boundary conditions. As seen in Problem 2.6, other discrete approximations to $\frac{\partial}{\partial\tau}+\epsilon_\alpha-\mu$ give inequivalent results emphasizing the fact that Eq. (2.65) rather than the continuum shorthand, Eq. (2.66) is the defining expression.

Finally, we evaluate the single-particle Green's function for non-interacting particles, $\mathcal{G}_0$. Let τ_α correspond to the time $q\frac{\beta}{M}$ and τ_r correspond to the time $r\frac{\beta}{M}$ for

integers q and r. Using Eq(2.67) for the non-interacting Hamiltonian, H_0, we obtain:

$$\begin{aligned}
\mathcal{G}_0(\alpha\tau_q|\gamma\tau_r) &= \frac{1}{Z_0}\mathrm{Tr}\left[Te^{-\int_0^\beta d\tau(H_0-\mu N)}a_\alpha(\tau_q)a_\gamma^\dagger(\tau_r)\right] \\
&= \frac{1}{Z_0}\lim_{M\to\infty}\int\prod_\delta\prod_{k=1}^{M}\frac{1}{\mathcal{N}}d\phi^*_{\delta,k}d\phi_{\delta,k}e^{-\sum_{j,k=1}^{M}\phi^*_{\delta,j}S^{(\delta)}_{jk}\phi_{\delta,k}}\phi_{\alpha,q}\phi^*_{\gamma,r} \\
&= \delta_{\alpha\gamma}\frac{\int\prod_k d\phi^*_k d\phi_k e^{-\sum_{j,k=1}^{M}\phi^*_j S^{(\alpha)}_{jk}\phi_k}\phi_q\phi^*_r}{\int\prod_k d\phi^*_k d\phi_k e^{-\sum_{j,k=1}^{M}\phi^*_j S^{(\alpha)}_{jk}\phi_k}} \\
&= \delta_{\alpha\gamma}\frac{\varsigma\partial^2}{\partial J^*_q\partial J_r}\left.\frac{\int\prod_k d\phi^*_k d\phi_k e^{-\sum_{j,k}\phi^*_j S^{(\alpha)}_{jk}\phi_k+\sum_i(J^*_i\phi_i+\phi^*_i J_i)}}{\int\prod_k d\phi^*_k d\phi_k e^{-\sum_{j,k}\phi^*_j S^{(\alpha)}_{jk}\phi_k}}\right|_{J=J^*=0} \\
&= \delta_{\alpha\gamma}\frac{\varsigma\partial^2}{\partial J^*_q\partial J_r}e^{\sum_{j,k}J^*_j S^{(\alpha)^{-1}}_{jk}J_k}\Big|_{J=J^*=0} \\
&= \delta_{\alpha\gamma}S^{(\alpha)^{-1}}_{qr} \quad .
\end{aligned} \tag{2.73}$$

The inverse of S in Eq. (2.70a), with a defined by Eq. (2.70b) is

$$S^{(\alpha)^{-1}} = \frac{1}{1-\varsigma a^M}\begin{bmatrix} 1 & \varsigma a^{M-1} & \varsigma a^{M-2} & \dots & \varsigma a \\ a & 1 & \varsigma a^{M-1} & & \varsigma a^2 \\ a^2 & a & 1 & & \\ \vdots & a^2 & a & & \vdots \\ & & a^2 & & \\ a^{M-3} & & & & \\ a^{M-2} & a^{M-3} & & & \varsigma a^{M-1} \\ a^{M-1} & a^{M-2} & a^{M-3} & \dots & 1 \end{bmatrix} . \tag{2.74}$$

Hence, for $q \geq r$

$$\begin{aligned}
\lim_{M\to\infty} S^{(\alpha)^{-1}}_{q,r} &= \lim_{M\to\infty}\frac{a^{q-r}}{1-\varsigma a^M} \\
&= \lim_{M\to\infty}\left(1-\frac{\beta}{M}(\epsilon_\alpha-\mu)\right)^{q-r}\left(1+\frac{\varsigma}{(1-\frac{\beta}{M}(\epsilon_\alpha-\mu))^{-M}-\varsigma}\right) \\
&= e^{-(\epsilon_\alpha-\mu)(\tau_q-\tau_r)}\left(1+\frac{\varsigma}{e^{\beta(\epsilon_\alpha-\mu)}-\varsigma}\right) \\
&= e^{-(\epsilon_\alpha-\mu)(\tau_q-\tau_r)}(1+\varsigma n_\alpha)
\end{aligned} \tag{2.75a}$$

where n_α is the familiar Boson or Fermion occupation probability

$$n_\alpha = \frac{1}{e^{\beta(\epsilon_\alpha-\mu)}-\varsigma} \quad . \tag{2.75b}$$

Similarly, for $q \leq r$

$$\begin{aligned}
\lim_{M\to\infty} S^{-1}_{q,r} &= \lim_{M\to\infty}\frac{\varsigma a^{M+q-r}}{1-\varsigma a^M} \\
&= \lim_{M\to\infty}\left(1-\frac{\beta}{M}(\epsilon_\alpha-\mu)\right)^{q-r}\frac{\varsigma}{(1-\frac{\beta}{M}(\epsilon_\alpha-\mu))^{-M}-\varsigma} \\
&= e^{-(\epsilon_\alpha-\mu)(\tau_q-\tau_r)}\varsigma n_\alpha \quad .
\end{aligned} \tag{2.76}$$

The two results specify the single-particle Green's function when $\tau_q \leq \tau_r$ and when $\tau_q \geq \tau_r$ respectively, so there only remains the case in which creation and annihilation operators act at equal physical times, as occurs for example whenever a second-quantized operator is evaluated at a specific time. Using the fact that the time-ordered product is defined to be equal to a normal-ordered product at equal time, the equal-time propagator may be obtained two equivalent ways. If the operator $a^\dagger_\alpha a_\beta$ is surrounded by evolution operators, subdivision of the interval in the usual way yields

$$\begin{aligned}
&e^{-\epsilon H}|\phi_k\rangle\langle\phi_k|a^\dagger_\alpha a_\beta e^{-\epsilon H}|\phi_{k-1}\rangle\langle\phi_{k-1}|\dots \\
&\qquad = e^{-\epsilon H}|\phi_k\rangle\left(\phi^*_{\alpha,k}\phi_{\beta,k-1}e^{-\epsilon H(\phi^*_k,\phi_{k-1})}+\mathcal{O}(\epsilon)\right)\langle\phi_{k-1}|\dots \quad .
\end{aligned} \tag{2.77a}$$

Thus, like the operators in H, the creation operator is evaluated one time step later than the annihilation operator, and the appropriate expression for the Green's function corresponding to equal times is Eq. (2.76) rather than Eq. (2.75). Alternatively, the time-ordered product may be written $T[a_\beta(\tau)a^\dagger_\alpha(\tau)] = \varsigma a^\dagger_\alpha(\tau)a_\beta(\tau) = a_\beta(\tau)a^\dagger_\alpha(\tau) - \delta_{\alpha\beta}$ in which case the evolution operator is expressed

$$\begin{aligned}
&|\phi_{k+1}\rangle\langle\phi_{k+1}|e^{-\epsilon H}a_\alpha|\phi_k\rangle\langle\phi_k|a^\dagger_\beta e^{-\epsilon H}|\phi_{k-1}\rangle\langle\phi_{k-1}|\dots \\
&\qquad = |\phi_{k+1}\rangle e^{-\epsilon H(\phi^*_{k+1},\phi_k)}\phi_{\alpha,k}\phi^*_{\beta,k}e^{-\epsilon H(\phi^*_k,\phi_{k-1})}\langle\phi_{k-1}|\dots
\end{aligned} \tag{2.77b}$$

and ϕ_α and ϕ^*_β are evaluated at equal times. Thus, $\langle Ta_\alpha(\tau)a^\dagger_\alpha(\tau)\rangle = S^{-1}_{r,r} - 1 = \varsigma n_\alpha$ as before.

Combining these results, the single-particle Green's function may be written

$$\begin{aligned}
\mathcal{G}_0(\alpha\tau|\alpha'\tau') &= \langle Ta_\alpha(\tau)a^\dagger_{\alpha'}(\tau')\rangle \\
&= \delta_{\alpha\alpha'}e^{-(\epsilon_\alpha-\mu)(\tau-\tau')}\{\theta(\tau-\tau'-\eta)(1+\varsigma n_\alpha)+\varsigma\theta(\tau'-\tau+\eta)n_\alpha\} \\
&= \delta_{\alpha\alpha'}g_\alpha(\tau-\tau'-\eta)
\end{aligned} \tag{2.78}$$

where the infinitesimal η serves as a reminder that the second term contributes at equal times. (A convenient mnemonic for the η is the fact that the time τ' associated with the creation operator is always shifted one time step later).

Although we have derived $\mathcal{G}$ carefully as the inverse of the discrete expression appearing in the exponent of the partition function, it may be obtained directly as the inverse of $(\partial_\tau + \epsilon_\alpha - \mu)$ by solving the differential equation

$$(\partial_\tau + \epsilon_\alpha - \mu)\mathcal{G}(\alpha\tau|\alpha\tau') = \delta(\tau-\tau') \tag{2.79a}$$

subject to the boundary condition

$$\mathcal{G}(\alpha\beta|\alpha\tau') = \varsigma\mathcal{G}(\alpha 0|\alpha\tau') \quad . \tag{2.79b}$$

The only ambiguity in the continuum derivation is the result at equal times. Whereas the discrete expression defining the functional integral produces the physical result at equal time, other discrete approximations to the continuum expression may be incorrect (see Problem 2.6).

2.3 PERTURBATION THEORY

In this section, we consider the case of a Hamiltonian which has been decomposed into the sum of a one-body operator H_0 and the residual Hamiltonian V, which in general may contain a one-body interaction as well as many-body interactions, and develop a systematic perturbation expansion in powers of V. The basis will be chosen to diagonalize $H_0 = \sum_\alpha \epsilon_\alpha a_\alpha^\dagger a_\alpha$ and we will write the normal-ordered many-body part as $V(a_\alpha^\dagger a_\beta^\dagger \ldots a_\gamma a_\delta \ldots)$ The starting point is to express the Grand partition function in terms of thermal averages defined with respect to H_0. To establish notation which will be used subsequently, we will define equivalent expressions in terms of operators and functional integrals. As in Eq. (2.67), creation and annihilation operators will be given a formal τ label denoting the time slice upon which they are defined. These operators $\{a_\alpha^\dagger(\tau), a_\alpha(\tau)\}$ are replaced by the coherent state variables $\{\psi_\alpha^*(\tau), \psi_\alpha(\tau)\}$ on the corresponding time slice in the functional integral and should not be confused with the Heisenberg operators $\{a_\alpha^{(H)\dagger}(\tau), a_\alpha^{(H)}\}$ defined in Eq. (2.23). The operator form of the partition function is written

$$\begin{aligned} Z &= \mathrm{Tr}\left[Te^{-\int_0^\beta d\tau\left(\sum_\alpha(\epsilon_\alpha-\mu)a_\alpha^\dagger(\tau)a_\alpha(\tau)+V(a_\alpha^\dagger(\tau)a_\beta^\dagger(\tau)\ldots a_\gamma(\tau)a_\delta(\tau)\right)}\right] \\ &= Z_0\langle e^{-\int_0^\beta d\tau V(a_\alpha^\dagger(\tau)a_\beta^\dagger(\tau)\ldots a_\gamma(\tau)a_\delta(\tau)}\rangle_0 \end{aligned} \tag{2.80a}$$

where the thermal average of an operator F is written

$$\begin{aligned} &\langle F(a_\alpha^\dagger(\tau_i)a_\beta^\dagger(\tau_j)\ldots a_\gamma(\tau_k)a_\delta(\tau_l)\ldots)\rangle_0 \\ &\quad = \frac{1}{Z_0}\mathrm{Tr}\left[Te^{-\int_0^\beta d\tau\sum_\alpha(\epsilon_\alpha-\mu)a_\alpha^\dagger(\tau)a_\alpha(\tau)}F(a_\alpha^\dagger(\tau_i)a_\beta^\dagger(\tau_j)\ldots a_\gamma(\tau_k)a_\delta(\tau_l)\ldots)\right] . \end{aligned} \tag{2.80b}$$

It is crucial to note that all the operators in F are subject to the time-ordering operator included in the definition of $\langle F\rangle_0$.

Equivalently, in terms of functional integrals, the partition function may be written

$$\begin{aligned} Z &= \int_{\substack{\psi(\beta)=\\ \varsigma\psi(0)}} \mathcal{D}(\psi_\alpha^*\psi_\alpha)e^{-\int_0^\beta d\tau\left(\sum_\alpha\psi_\alpha^*(\tau)(\partial_\tau+\epsilon_\alpha-\mu)\psi_\alpha(\tau)+V(\psi_\alpha^*(\tau),\psi_\beta^*(\tau)\ldots,\psi_\gamma(\tau),\psi_\delta(\tau)\ldots)\right)} \\ &= Z_0\langle e^{-\int_0^\beta d\tau V(\psi_\alpha^*(\tau),\psi_\beta^*(\tau)\ldots,\psi_\gamma(\tau),\psi_\delta(\tau)\ldots)}\rangle_0 \end{aligned} \tag{2.81a}$$

where the thermal average is defined

$$\begin{aligned} &\langle F(\psi_\alpha^*(\tau_i),\psi_\beta^*(\tau_j)\ldots\psi_\gamma(\tau_k)\psi_\delta(\tau_l))\rangle_0 \\ &\quad = \frac{1}{Z_0}\int_{\psi(\beta)=\varsigma\psi(0)} \mathcal{D}(\psi_\alpha^*\psi_\alpha)e^{-\sum_\alpha\int_0^\beta d\tau\psi_\alpha^*(\partial_\tau+\epsilon_\alpha-\mu)\psi_\alpha} \\ &\quad \times F(\psi_\alpha^*(\tau_i)\psi_\beta^*(\tau_j)\ldots\psi_\gamma(\tau_k)\psi_\delta(\tau_l)\ldots) \quad . \end{aligned} \tag{2.81b}$$

Note that the time-ordering which was explicit for operators is implicit because the functional integral always represents time-ordered products.

The partition function of the non-interacting system, Z_0, appearing in Eqs. (2.58) and (2.81) may be written

$$Z_0 = \mathrm{Tr}\left[Te^{-\int_0^\beta d\tau\sum_\alpha(\epsilon_\alpha-\mu)a_\alpha^\dagger(\tau)a_\alpha(\tau)}\right] \tag{2.82a}$$

$$= \int_{\psi(\beta)=\varsigma\psi(0)} \mathcal{D}(\psi_\alpha^*\psi_\alpha)e^{-\sum_\alpha\int_0^\beta d\tau\psi_\alpha^*(\tau)(\partial_\tau+\epsilon_\alpha-\mu)\psi_\alpha(\tau)} \quad . \tag{2.82b}$$

Because of the equivalence of Eqs. (2.80) and (2.81), we will henceforth pass freely between thermal averages $\langle\ \rangle_0$ of operators and of complex or Grassman variables. Note that analogous expression will also be introduced later for thermal averages $\langle\ \rangle$ defined with respect to the full Hamiltonian by replacing H_0 by H in Eqs. (2.80b) and (2.81b).

The perturbation expansion is obtained by expanding Eq. (2.81a) in a power series

$$\begin{aligned} \frac{Z}{Z_0} &= \sum_{n=0}^\infty \frac{(-1)^n}{n!}\int_0^\beta d\tau_1\ldots d\tau_n \\ &\quad \langle V(\psi_\alpha^*(\tau_1)\ldots,\psi_\gamma(\tau_1)\ldots)\ldots V(\psi_\alpha^*(\tau_n)\ldots,\psi_\gamma(\tau_n)\ldots)\rangle_0 \quad . \end{aligned} \tag{2.83}$$

We will proceed by deriving a form of Wick's theorem to evaluate the thermal averages of the products of ψ^* and ψ which arise in Eq. (2.83) and then develop a systematic set of rules for constructing Feynman diagrams.

WICK'S THEOREM

In the form we will use it, Wick's theorem corresponds to the following identity for the integral of a product of a polynomial with a Gaussian

$$\frac{\int\mathcal{D}(\psi^*\psi)\psi_{i_1}\psi_{i_2}\ldots\psi_{i_n}\psi_{j_n}^*\ldots\psi_{j_2}^*\psi_{j_1}^*e^{-\sum_{ij}\psi_i^*M_{ij}\psi_j}}{\int\mathcal{D}(\psi^*\psi)e^{-\sum_{ij}\psi_i^*M_{ij}\psi_j}} = \sum_P\varsigma^P M^{-1}_{i_{Pn},j_n}\ldots M^{-1}_{i_{P1},j_{P1}} \tag{2.84}$$

where, as usual (ψ^*,ψ) denote complex or Grassman variables, $\mathcal{D}(\psi^*\psi)$ is the appropriate measure, and we have simplified the notation by letting j denote the state and

time labels. We will first prove this identity and then relate it to evaluation of Green's functions, thermal averages, and the traditional statement of Wick's theorem.

The identity Eq. (2.84) is a generalization of the result Eq. (2.73) and may be derived in the same way using the generating function

$$G(J^*,J) = \frac{\int \mathcal{D}(\psi^*\psi) e^{-\sum_{ij}\psi_i^* M_{ij}\psi_j + \sum_i (J_i^*\psi_i + \psi_i^* J_i)}}{\int \mathcal{D}(\psi^*\psi) e^{-\sum_{ij}\psi_i^* M_{ij}\psi_j}} = e^{\sum_{ij} J_i^* M_{ij}^{-1} J_j} \quad . \tag{2.85}$$

Differentiation of the first line of Eq. (2.85) with respect to the sources J and J^* yields

$$\left.\frac{\delta^{2n} G}{\delta J_{i_1}^* \dots \delta J_{i_n}^* \delta J_{j_n} \dots \delta J_{j_1}}\right|_{\substack{J=0\\J^*=0}} = (\varsigma)^n \frac{\int \mathcal{D}(\psi^*\psi) e^{-\sum \psi_i^* M_{ij}\psi_j} \psi_{i_1} \dots \psi_{i_n} \psi_{j_n}^* \dots \psi_{j_1}^*}{\int \mathcal{D}(\psi^*\psi) e^{-\sum \psi_i^* M_{ij}\psi_j}} \quad . \tag{2.86}$$

Note that in deriving this result, we used the fact that all the terms in the exponent are even in the J's and ψ's and thus commute with ψ, ψ^*, J and J^* and the fact that an odd number of interchanges is required for each differentiation with respect to J. Differentiation of the second line of Eq. (2.85) yields

$$\begin{aligned}
&\frac{\delta^{2n}}{\delta J_{i_1}^* \dots \delta J_{i_n}^* \delta J_{j_n} \dots \delta J_{j_1}} \left(e^{\sum_{ij} J_i^* M_{ij} J_i}\right)\Big|_{\substack{J^*=0\\J=0}} \\
&= \varsigma^n \frac{\delta^n}{\delta J_{i_1}^* \dots \delta J_{i_n}^*} \left(\sum_{k_n} J_{k_n}^* M_{k_n j_n}^{-1}\right) \dots \left(\sum_{k_1} J_{k_1}^* M_{k_1 j_1}^{-1}\right) e^{\sum_{ij} J_i^* M_{ij}^{-1} J_j}\Big|_{\substack{J^*=0\\J=0}} \\
&= \varsigma^n \sum_P \varsigma^P M_{i_{Pn} j_n}^{-1} \dots M_{i_{P1} j_1}^{-1} \quad .
\end{aligned} \tag{2.87}$$

Equating the two expressions Eqs. (2.86) and (2.87) proves Eq. (2.84).

We now apply this identity to the case of physical interest by defining M_{ij} to be the discrete matrix representing $(\partial_t + H_0 - \mu)$, Eq. (2.69), replacing ψ_j by $\psi_{\alpha,k}$, where α denotes the basis states in the diagonal representation and k denotes the time point on a mesh of M points with $\Delta\tau = \frac{\beta}{M}$. As shown in the preceding section, M_{ij}^{-1} is then the single particle Green's function, Eq. (2.78):

$$\begin{aligned}
\mathcal{G}_0(\alpha_1\tau_1|\alpha_2\tau_2) &= \frac{\int \mathcal{D}(\psi^*\psi)\psi_{\alpha_1}(\tau_1)\psi_{\alpha_2}^*(\tau_2) e^{-\int d\tau \sum_\alpha \psi_\alpha^*(\partial_\tau + \epsilon_\alpha - \mu)\psi_\alpha}}{\int \mathcal{D}(\psi^*\psi) e^{-\int d\tau \sum_\alpha \psi_\alpha(\partial_\tau + \epsilon_\alpha - \mu)\psi_\alpha}} \\
&= (\partial_\tau + \epsilon_\alpha - \mu)^{-1}_{\alpha_1\tau_1;\alpha_2\tau_2} \\
&\equiv \delta_{\alpha_1\alpha_2} g_{\alpha_1}(\tau_1 - \tau_2 - \eta) \quad .
\end{aligned} \tag{2.88}$$

The identity (2.84) then states that the n-particle Green's function for a non-interacting system is the sum of all permutations of the products of one-particle Green's functions

$$\begin{aligned}
&\mathcal{G}^{(n)}(\alpha_1\tau_1 \dots \alpha_n\tau_n|\alpha_1'\tau_1' \dots \alpha_n'\tau_n') \\
&\quad = \sum_P \varsigma^P \delta_{\alpha_{P1},\alpha_1'} \dots \delta_{\alpha_{Pn}\alpha_n'} g_{\alpha_1'}(\tau_{P1} - \tau_1') \dots g_{\alpha_n'}(\tau_{Pn} - \tau_n') \quad .
\end{aligned} \tag{2.89}$$

We may establish contact with the traditional statement of Wick's theorem by defining contractions of time-dependent operators. Let $\tilde{a}_\alpha(\tau)$ denote any creation operator $a_\alpha^\dagger(\tau)$ or annihilation operator $a_\alpha(\tau)$ and let $\tilde{\psi}_\alpha(\tau)$ denote the corresponding complex or Grassman variable $\psi_\alpha^*(\tau)$ or $\psi_\alpha(\tau)$. A contraction is then defined as

$$\overbrace{\tilde{a}_\alpha(\tau)\tilde{a}_{\alpha'}(\tau')} = \langle T[\tilde{a}_\alpha(\tau)\tilde{a}_{\alpha'}(\tau')]\rangle_0 = \langle \tilde{a}_\alpha(\tau)\tilde{a}_{\alpha'}(\tau')\rangle_0 \tag{2.90}$$

where the thermal average is defined by Eq. (2.80) and the explicit T-product may be omitted because the operators are necessarily time-ordered by the definition of the thermal average. An equivalent definition is given by

$$\overbrace{\tilde{\psi}_\alpha(\tau)\tilde{\psi}_{\alpha'}(\tau')} = \langle \tilde{\psi}_\alpha(\tau)\tilde{\psi}_{\alpha'}(\tau')\rangle_0 \tag{2.91}$$

where the thermal average is given by Eq. (2.81). From Eq. (2.88) we obtain

$$\begin{aligned}
\overbrace{a_\alpha(\tau)a_{\alpha'}^\dagger(\tau')} &= \overbrace{\psi_\alpha(\tau)\psi_{\alpha'}^*(\tau')} \\
&= \delta_{\alpha\alpha'} g_\alpha(\tau - \tau')
\end{aligned} \tag{2.92a}$$

and

$$\begin{aligned}
\overbrace{a_{\alpha'}^\dagger(\tau')a_\alpha(\tau)} &= \overbrace{\psi_{\alpha'}^*(\tau')\psi_\alpha(\tau)} \\
&= \varsigma\delta_{\alpha\alpha'} g_\alpha(\tau - \tau') \quad .
\end{aligned} \tag{2.92b}$$

Because the expectation value of two creation or annihilation operators is zero in any state of definite particle number, or by explicit integration of the corresponding Gaussian integral, the following contractions vanish:

$$\overbrace{a_\alpha^\dagger(\tau)a_{\alpha'}^\dagger(\tau')} = \overbrace{\psi_\alpha^*(\tau)\psi_{\alpha'}^*(\tau')} = 0 \tag{2.92c}$$

and

$$\overbrace{a_\alpha(\tau)a_{\alpha'}(\tau')} = \overbrace{\psi_\alpha(\tau)\psi_{\alpha'}(\tau')} = 0 \quad . \tag{2.92d}$$

Given these definitions, note that with $M \equiv (\partial_t + H_0 - \mu)$ the left hand side of the identity Eq. (2.84) is $\langle \psi_{i_1}\psi_{i_2} \dots \psi_{i_n}\psi_{j_n}^* \dots \psi_{j_2}^*\psi_{j_1}^*\rangle_0$ and each factor in the right hand side corresponds to a contraction $\psi_i\psi_j^* = (\partial_\tau + H_0 - \mu)_{ij}^{-1}$. Thus, in this case, the thermal average is given by the sum over all complete sets of contractions, where a complete contraction is a configuration in which each ψ is contracted with a ψ^* and the overall sign is specified by ς^P where P is the permutation such that $\psi_{i_{Pn}}$ is contracted with $\psi_{j_n}^*$. If one considered the expectation value of a product of an unequal number of ψ's and ψ^*'s, it would still be equal to the sum of all contractions since the complete expectation value would vanish and at least one contraction in each complete set of contractions would also vanish. Thus, the general statement of Wick's theorem, using the notation of Eqs. (2.90) and (2.91) to denote creation or annihilation operators, is the following:

$$\begin{aligned}
\langle T[\tilde{a}_{\alpha_1}(\tau_1) \dots \tilde{a}_{\alpha_n}(\tau_n)]\rangle_0 &= \langle \tilde{\psi}_{\alpha_1}(\tau_1) \dots \tilde{\psi}_{\alpha_n}(\tau_n)\rangle_0 \\
&= \sum \text{all complete contractions} \quad .
\end{aligned} \tag{2.93}$$