14

The statistical mechanics connection

Models from quantum mechanics can be converted into statistical mechanics systems through the Wick rotation $t \rightsquigarrow -\mathrm{i}t$. Within quantum field theory this technique has been very powerful, both in proving qualitative properties and as a computational tool. Besides these more practical aspects, the statistical mechanics formulation is an additional source of intuition which cannot so easily be extracted from the Schrödinger differential equation. The price to pay is that, in essence only ground state properties can be handled. Truly time-dependent problems must be treated in physical time. For charges interacting with the Maxwell field the Wick rotation is equally attractive. There is one additional bonus: since the field Hamiltonian is quadratic and since the coupling to the field is linear, as first observed by Feynman, the Gaussian integration over the Maxwell field can be done explicitly. This results in a fairly concise statistical-mechanical description for the particles.

In Euclidean language the possible paths of the charge and the fields become fluctuating quantities. To distinguish in notation we use $t \mapsto q_t$ for a random path of the charge and $t \mapsto A_t(x)$ for a random history of the transverse vector field. $\mathbb{E}(\cdot)$ refers to expectation with respect to the measure of integration, either specified through the context or indicated by a subscript. Sometimes we also use the statistical mechanics shorthand $\langle \cdot \rangle$ for averages.

14.1 Functional integral representation

For a single particle, subject to the potential $V(x)$, the imaginary time Schrödinger equation is, setting $\hbar = 1 = m$,

$$\partial_t \psi = -H_{\mathrm{p}} \psi \,, \quad H_{\mathrm{p}} = -\frac{1}{2}\Delta + V \tag{14.1}$$

and its solution for $t \geq 0$ is constructed through the Trotter product formula as

$$(\mathrm{e}^{-tH_{\mathrm{p}}}\psi)(x) = \lim_{n\to\infty} (\mathrm{e}^{t\Delta/2n}\mathrm{e}^{-tV/n})^n \psi(x) \,. \tag{14.2}$$

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We recognize $\exp[\frac{1}{2}t\Delta]$ as the transition probability for a Brownian motion, whose paths will be denoted here by $t \mapsto q_t$. Brownian motion is a Gaussian process and therefore defined through the mean and covariance. Explicitly,

$$\mathbb{E}(q_t) = 0\,, \quad \mathbb{E}(q_{s\alpha} q_{t\beta}) = \delta_{\alpha\beta} \min(s,t)\,. \tag{14.3}$$

If the Brownian motion starts at x, we indicate the start point as a subscript in the expectation and have $\mathbb{E}_x(q_t) = x$, $\mathbb{E}_x((q_s - x)_\alpha (q_t - x)_\beta) = \delta_{\alpha\beta} \min(s,t)$, $\alpha, \beta = 1, 2, 3$. In particular the transition probability is obtained as

$$\mathbb{P}_x(\{q_t \in \mathrm{d}^3 y\}) = (2\pi t)^{-3/2} \exp[-(y-x)^2/2t] \mathrm{d}^3 y = (\mathrm{e}^{t\Delta/2})(x,y) \mathrm{d}^3 y\,. \tag{14.4}$$

Writing out (14.2) in position space representation, one infers the Feynman–Kac formula

$$(\mathrm{e}^{-tH_{\mathrm{p}}}\psi)(x) = \mathbb{E}_x\Big(\exp\Big[-\int_0^t \mathrm{d}s\, V(q_s) \Big] \psi(q_t) \Big)\,. \tag{14.5}$$

The Brownian motion path has acquired a non-Gaussian weight, which is the exponential of the potential energy integrated along the path q_t.

The statistical mechanics connection becomes more obvious upon discretizing time in units of τ. We set $\phi_n = q_{n\tau}$, $\phi_n \in \mathbb{R}^3$. Then, in approximation, (14.5) reads

$$\begin{aligned} &\frac{1}{Z} \int \mathrm{d}^3\phi_0 \ldots \mathrm{d}^3\phi_N\, \delta(\phi_0 - x) \exp\Big[-\frac{1}{2\tau} \sum_{j=0}^{N-1} (\phi_{j+1} - \phi_j)^2 \Big] \\ &\quad \times \exp\Big[-\tau \sum_{j=1}^{N} V(\phi_j) \Big] \psi(\phi_N)\,, \end{aligned} \tag{14.6}$$

$N\tau = t$. The statistical mechanics model lives on a one-dimensional lattice and has at each site a continuous "spin" with three components. The first exponential is a quadratic nearest-neighbor interaction and, except for the normalization, represents a discrete-time Gaussian random walk in $\mathbb{R}^3$. The potential can be combined with the Lebesgue measure as $\exp[-\tau V(\phi_j)]\mathrm{d}^3\phi_j$ and thus provides a non-Gaussian single-site measure.

For (14.5) to make sense one needs some minimal conditions on V to ensure that the expectation is defined. An obvious sufficient condition is to have $V \geq c_0 > -\infty$. Equation (14.5) indicates that very roughly there are three families of potentials: (i) *Binding*, V increases at infinity. Under the measure in (14.5) q_t has in essence bounded fluctuations. For $t \to \infty$ the path measure for q_t becomes a stationary diffusion process. (ii) *No binding*, e.g. a repulsive potential decaying to zero at infinity or a bounded periodic potential. A typical path q_t fluctuates and diffuses to infinity as a Brownian motion with some effective diffusion coefficient. (iii) *Local binding*, like an attractive square-well potential. For the purpose

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of discussion let us set the potential as λV with V attractive near the origin and decaying to zero at infinity. For large λ the potential dominates and q_t is confined as a stationary diffusion process. As λ decreases, q_t makes longer and longer excursions until it unbinds at some critical λ_c. For $\lambda < \lambda_c$ the Brownian motion dominates. Since Brownian motion is recurrent in dimension $d = 1, 2$, one has $\lambda_c = 0$, whereas for $d = 3$ generically $\lambda_c > 0$.

It is of use to translate the path properties of the particle to spectral properties of the particle Hamiltonian $H_p = -\frac{1}{2}\Delta + V$. We denote by Σ the continuum edge of H_p and, if it exists, by ψ_0 the unique ground state of H_p, i.e. $H_p\psi_0 = E_0\psi_0$. In case (i) the spectrum of H_p is purely discrete, formally $\Sigma = \infty$. In the second case H_p has a purely continuous spectrum and no eigenvalues. For a locally binding potential which decays to zero at infinity, case (iii), the continuum edge is $\Sigma = 0$. For sufficient attraction there are bound states with an energy below Σ, in particular $E_0 < 0$. In dimension $d = 1, 2$ an arbitrarily weak attraction results in a bound state, whereas for $d \geq 3$ a minimal strength is required. As is well understood, there is more complicated spectral behavior around with various borderline cases. For our purposes the schematic classification above will suffice.

Our goal is to extend the Feynman–Kac formula (14.5) to e^{-tH} with H the Pauli–Fierz Hamiltonian. This will be done in two steps. Firstly we study a one-particle Hamiltonian including an external vector potential, and secondly we write e^{-tH_f} in terms of a suitable Gaussian measure. Combining both elements yields the desired generalization.

Let us assume then that the quantum particle is subject to a magnetic field and denote the corresponding vector potential by $a(x)$, to distinguish from the fluctuating vector potential A_t used later on. The imaginary time Schrödinger equation becomes

$$\partial_t \psi = -H_p \psi \,, \quad H_p = \frac{1}{2}(-i\nabla - a)^2 + V \,. \tag{14.7}$$

Then, as before, we represent e^{-tH_p} through the Trotter product formula. The vector potential yields a term proportional to $\dot{q}$, as can be guessed from the corresponding classical action. More precisely one obtains

$$(e^{-tH_p}\psi)(x) = \mathbb{E}_x\Big(\exp\Big[-i\int_0^t dq_s \cdot a(q_s) - \frac{i}{2}\int_0^t ds\, \nabla \cdot a(q_s) - \int_0^t ds\, V(q_s)\Big]\psi(q_t)\Big) \,. \tag{14.8}$$

The stochastic integral appearing in (14.8) is defined as Ito integral, which means that the discretization of $a(x)$ is evaluated at the left end point,

$$\int_0^t dq_s \cdot a(q_s) = \lim_{n\to\infty} \sum_{m=1}^{nt} a(q_{(m-1)/n}) \cdot (q_{m/n} - q_{(m-1)/n}) \,. \tag{14.9}$$

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This limit exists almost surely with respect to Brownian motion. Through the Ito convention one picks up in (14.8) the additional term containing $\nabla \cdot a$. It disappears, if in (14.9) we were to use the, in our context perhaps more natural, Feynman–Stratonovich midpoint rule where $a(q_{(m-1)/n})$ is replaced by $\frac{1}{2}(a(q_{m/n}) + a(q_{(m-1)/n}))$. Note that in the Coulomb gauge the stochastic integral does not depend on the particular choice of the rule for the discretization, since $\nabla \cdot a = 0$.

On a purely formal level, following Feynman, the quantum propagator is written as a sum over all paths from x' to x in the time span t "weighted" by the exponential of the classical action,

$$(\mathrm{e}^{-\mathrm{i}H_{\mathrm{p}}t})(x, x') = \int \prod_{0\le s\le t} \mathrm{d}^3 q_s \delta(q_0 - x')\delta(q_t - x) \exp\Big[\mathrm{i}\int_0^t \mathrm{d}s L(q_s, \dot{q}_s)\Big] \tag{14.10}$$

with the classical Lagrangian $L(q, \dot{q}) = \frac{1}{2}\dot{q}^2 - V(q) + \dot{q} \cdot a(q)$. Note that compared to the right side of (14.8) the role of x and x' has been interchanged. Upon Wick rotation $t \rightsquigarrow -\mathrm{i}t$ and time reversal $q_s \rightsquigarrow q_{t-s}$ (14.10) becomes

$$\begin{aligned}(\mathrm{e}^{-tH_{\mathrm{p}}})(x, x') = \int \prod_{0\le s\le t} \mathrm{d}^3 q_s \delta(q_0 - x)\delta(q_t - x') \\ \times \exp\Big[-\int_0^t \mathrm{d}s \big(\frac{1}{2}\dot{q}_s^2 + V(q_s) + \mathrm{i}\dot{q}_s \cdot a(q_s)\big)\Big]. \end{aligned} \tag{14.11}$$

One recognizes the potential term and the stochastic integral $-\mathrm{i}\int_0^t \mathrm{d}s \dot{q}_s \cdot a(q_s)$ with the mid point rule. The exponential of the kinetic term combines with the infinite-product Lebesgue measure to Brownian motion, denoted by $\mathbb{E}_x$ in (14.8), which starts at x according to the factor $\delta(q_0 - x)$.

We turn to the functional integral for the Maxwell field, which we can think of as an infinite collection of harmonic oscillators. Let us first recall the single harmonic oscillator with Hamiltonian

$$H = \frac{1}{2}\big(-\partial_x^2 + \omega^2 x^2 - \omega\big) \tag{14.12}$$

as a differential operator acting on $L^2(\mathbb{R}, \mathrm{d}x)$. It has the normalized eigenvectors $|n\rangle$, $n = 0, 1, \ldots$, i.e.

$$H|n\rangle = \varepsilon_n |n\rangle\,, \quad \varepsilon_n = \omega n\,. \tag{14.13}$$

$|0\rangle$ is the ground state of H. In the position representation $H\psi_0 = 0$ with $\psi_0(x)^2 = \sqrt{\omega/\pi}\mathrm{e}^{-\omega x^2}$. Thus, alternatively we can use the linear span of the $|n\rangle$'s as the Hilbert space of states. This corresponds to the Fock space $\mathcal{F}$ over

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the one-particle space $\mathbb{C}$, which means $\psi \in \mathcal{F}$ is of the form $\psi = (\psi_0, \psi_1, \dots)$, $\psi = \sum_{n=0}^{\infty} \psi_n |n\rangle$. A further, as it will turn out natural, choice is the Hilbert space $\mathcal{H}_0 = L^2(\mathbb{R}, \psi_0(x)^2 \mathrm{d}x)$ with weight given by the square of the ground state wave function.

Of course, these Hilbert spaces are unitarily equivalent. Of interest is the unitary map from $\mathcal{F}$ to $\mathcal{H}_0$ which is achieved through the Wick ordering of polynomials. We regard x as a random variable on $\mathbb{R}$ equipped with the normalized Gaussian measure $\psi_0(x)^2 \mathrm{d}x$. Then, denoting expectation by $\langle \cdot \rangle$, the Wick order of x is defined recursively through $:x^0: = 1$, $\partial_x :x^n: = n :x^{n-1}:$, and $\langle :x^n: \rangle = 0$, $n = 1, 2, \dots$. Note that the Wick order depends both on the random variable and on the underlying measure. Thus $:1: = 1, :x: = x - \langle x \rangle = x, :x^2: = x^2 - 2\langle x \rangle x - \langle x^2 \rangle + 2\langle x \rangle^2 = x^2 - (1/2\omega)$, etc., in our case. Let P_n denote the n-th Hermite polynomial,

$$P_n(x) = \sum_{j=0}^{[n/2]} \frac{n!}{(n-2j)!\, j!} (-\tfrac{1}{2})^j x^{n-2j} \,, \tag{14.14}$$

with $[n]$ the integer part. Then the Wick-ordered mononomial of order n is given by

$$:x^n: = (2\omega)^{-n/2} P_n(\sqrt{2\omega} x) \,. \tag{14.15}$$

One has

$$\langle :x^n: :x^m: \rangle = \langle :x^n: , :x^m: \rangle_{\mathcal{H}_0} = (2\omega)^{-n} n! \delta_{mn} \,. \tag{14.16}$$

By linearity Wick order extends to all finite polynomials. Let us also introduce

$$a^* = \frac{1}{\sqrt{2\omega}} (\omega x - \partial_x) \,, \quad a = \frac{1}{\sqrt{2\omega}} (\omega x + \partial_x) \tag{14.17}$$

as creation and annihilation operators of the harmonic oscillator. Their Wick order means that all annihilation operators are moved to the right, e.g. $:aa^*: = a^* a$. Then

$$:\Big(\frac{1}{\sqrt{2\omega}} (a^* + a) \Big)^n : |0\rangle = (2\omega)^{-n/2} \sqrt{n!} |n\rangle \,. \tag{14.18}$$

Comparing with (14.16) the map U from $\mathcal{F}$ to $\mathcal{H}_0$ should be defined through

$$:\Big(\frac{1}{\sqrt{2\omega}} (a^* + a) \Big)^n : |0\rangle \mapsto :x^n: \tag{14.19}$$

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and extended by linearity. By the very construction the closure of U as a linear map $\mathcal{F} \to \mathcal{H}_0$ is then unitary. Note that e^{-tH} is implemented as

$$U\mathrm{e}^{-tH}U^{-1}:x^n:=:(\mathrm{e}^{-\omega t}x)^n:=\mathrm{e}^{-n\omega t}:x^n:\,. \tag{14.20}$$

Through the Feynman–Kac formula (14.5) we boost (14.12) to a Gaussian stochastic process denoted by x_t. It takes real values, is stationary in time, has mean zero, and covariance

$$\mathbb{E}(x_t x_s)=\frac{1}{2\omega}\mathrm{e}^{-\omega|t-s|}\,. \tag{14.21}$$

We recognize x_t as the stationary Ornstein–Uhlenbeck process governed by the stochastic differential equation

$$\mathrm{d}x_t=-\omega x_t\mathrm{d}t+\mathrm{d}b_t\,, \tag{14.22}$$

where b_t is standard one-dimensional Brownian motion. Note that

$$\mathbb{E}(f(x_t))=\mathbb{E}(f(x_0))=\langle\psi_0,\,f\psi_0\rangle=\langle 1,\,f\rangle_{\mathcal{H}_0}=\int \mathrm{d}x\,\psi_0(x)^2 f(x)\,, \tag{14.23}$$

$$\mathbb{E}(f(x_t)g(x_s))=\langle\psi_0,\,f\mathrm{e}^{-|t-s|H}g\psi_0\rangle=\langle f,\,\mathrm{e}^{|t-s|L}g\rangle_{\mathcal{H}_0}\,, \tag{14.24}$$

where we used the similarity transformation

$$\psi_0^{-1}\mathrm{e}^{-tH}\psi_0=\mathrm{e}^{tL}\,,\quad t\geq 0\,, \tag{14.25}$$

with L the generator of the Ornstein–Uhlenbeck process x_t,

$$L=-\omega x\partial_x+\tfrac{1}{2}\partial_x^2\,. \tag{14.26}$$

According to (14.23) the Ornstein–Uhlenbeck process x_t has $\psi_0(x)^2$ as stationary measure. With probability one $t\mapsto x_t$ is continuous and we may choose $C(\mathbb{R},\mathbb{R})$, the space of all continuous functions over $\mathbb{R}$, as path space. In fact, x_t has in essence bounded fluctuations and increases at most logarithmically for large t.

The point of our exercise is that it carries over essentially verbatim to the infinite-dimensional setting, except for the flat Hilbert space $L^2(\mathbb{R},\mathrm{d}x)$. H_f plays the role of the harmonic oscillator. The boson Fock space over the transverse vector fields $L^2_\perp(\mathbb{R}^3,\mathbb{R}^3)$ plays the role of the Fock space over $\mathbb{C}$. The Ornstein–Uhlenbeck process x_t is replaced by the infinite-dimensional Ornstein–Uhlenbeck process $A_t(x)$. Let us start with the latter. $A_t(x)$ is a Gaussian process with mean zero and covariance

$$\mathbb{E}\big(A_{t\alpha}(x)A_{t'\alpha'}(x')\big)=(2\pi)^{-3}\int \mathrm{d}^3k\mathrm{e}^{\mathrm{i}k\cdot(x-x')}Q^\perp_{\alpha\alpha'}(k)\frac{1}{2\omega}\mathrm{e}^{-\omega|t-t'|}\,, \tag{14.27}$$

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$\alpha, \alpha' = 1, 2, 3$. Because of the transverse projection $Q^{\perp}_{\alpha\alpha'}(k) = \delta_{\alpha\alpha'} - \widehat{k}_\alpha \widehat{k}_{\alpha'}$ the covariance (14.27) implies that

$$\nabla \cdot A_t = 0 \tag{14.28}$$

almost surely. $A_t(x)$ becomes a proper Gaussian random variable once it is integrated over the real test function f,

$$A_t(f) = \sum_{\alpha=1}^{3} \int \mathrm{d}^3 x f_\alpha(x) A_{t\alpha}(x) \,. \tag{14.29}$$

From (14.27) we conclude that

$$\mathbb{E}\big(A_t(f)^2\big) = \int \mathrm{d}^3 k (2\omega)^{-1} \widehat{f}^* \cdot Q^{\perp} \widehat{f} \,. \tag{14.30}$$

Thus $A_t(f)$ has a bounded variance provided $\| f/\sqrt{\omega} \|_{\mathfrak{h}} < \infty$.

In quantum field theory Lorentz invariance is of central importance; this becomes more evident by treating time and space on an equal footing. We thus Fourier transform in (14.27) also with respect to t and obtain

$$\mathbb{E}\big(\widehat{A}_\alpha(k_0, k)^* \widehat{A}_{\alpha'}(k_0', k')\big) = \delta(k - k')\delta(k_0 - k_0') Q^{\perp}_{\alpha\alpha'}(k)(k^2 + k_0^2)^{-1} \,, \tag{14.31}$$

which is more symmetric. However, fixing the Coulomb gauge spoils full rotation invariance in $\mathbb{R}^4$.

In our context time is singled out and we prefer to think of $t \mapsto A_t$ as a stochastic process with values in the transverse vector fields. Most conveniently, we regard A_t as the element of a Hilbert space $\mathcal{K}'$, which is chosen such that $t \mapsto A_t$ is continuous in t. $A_t(x)$ is somewhat singular in x, which has to be balanced by defining the norm of the Hilbert space $\mathcal{K}'$ through the inner product

$$\langle f, g \rangle_{\mathcal{K}'} = \sum_{\lambda=1,2} \int \mathrm{d}^3 k \widehat{f}(k, \lambda)^* \omega^{1/2} (-\Delta_k + k^2)^{-\kappa} \omega^{1/2} \widehat{g}(k, \lambda) \tag{14.32}$$

with some $\kappa \geq 0$. The predual Hilbert space is denoted by $\mathcal{K}$. It has the inner product

$$\langle f, g \rangle_{\mathcal{K}} = \sum_{\lambda=1,2} \int \mathrm{d}^3 k \widehat{f}(k, \lambda)^* \omega^{-1/2} (-\Delta_k + k^2)^{\kappa} \omega^{-1/2} \widehat{g}(k, \lambda) \,. \tag{14.33}$$

Lemma 14.1 (Regularity properties for sample paths of the Ornstein–Uhlenbeck process). *We regard the Ornstein–Uhlenbeck process $A_t(x)$ with covariance (14.27) as taking values in the Hilbert space $\mathcal{K}'$ with $\kappa > \frac{7}{2}$. Then $t \mapsto A_t \in \mathcal{K}'$ is almost surely (norm) continuous. The path space of the Ornstein–Uhlenbeck*

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process can be taken as $C(\mathbb{R}, \mathcal{K}')$, the space of continuous functions with values in $\mathcal{K}'$.

Proof: The Ornstein–Uhlenbeck process A_t is Markov and time reversible. A general estimate for such processes gives

$$\mathbb{E}\Big(\sup_{0\le t\le T} A_t(f)^2\Big) \le 3\mathbb{E}\big(A_0(f)^2\big) + 72T\mathcal{D}\big(A_0(f), A_0(f)\big)\,, \tag{14.34}$$

where $\mathcal{D}$ is the Dirichlet form defined through

$$\mathcal{D}\big(A_0(f), A_0(f)\big) = \lim_{t\to 0}\frac{1}{t}\Big(\mathbb{E}\big(A_t(f)A_0(f)\big) - \mathbb{E}\big(A_0(f)^2\big)\Big)\,. \tag{14.35}$$

Therefore

$$\mathbb{E}\Big(\sup_{0\le t\le T} A_t(f)^2\Big) \le c_0 \sum_{\lambda=1,2}\int \mathrm{d}^3k\,|\widehat{f}(k,\lambda)|^2(1+\omega^{-1})\,. \tag{14.36}$$

The eigenfunctions of $(-\Delta_k + k^2)$ are the Hermite functions h_n, $n \in \mathbb{N}^3$, with eigenvalue $\lambda_n = 1 + 2\sum_{\alpha=1}^3 n_\alpha$. Therefore

$$\begin{aligned}\mathbb{E}\Big(\sup_{0\le t\le T}\|A_t\|^2_{\mathcal{K}'}\Big) &= \mathbb{E}\Big(\sup_{0\le t\le T}\sum_{n\in\mathbb{N}^3}(\lambda_n)^{-\kappa}A_t(\sqrt{\omega}h_n)^2\Big)\\ &\le c_0\sum_{n\in\mathbb{N}^3}(\lambda_n)^{-\kappa}\int \mathrm{d}^3k\,|\widehat{h}_n(k)|^2(1+\omega)\,.\end{aligned} \tag{14.37}$$

Using operator monotonicity as $(k^2)^{1/2} \le (-\Delta_k + k^2)^{1/2}$ yields the bound

$$c_0\sum_{n\in\mathbb{N}^3}(\lambda_n)^{-\kappa+\frac{1}{2}}\,, \tag{14.38}$$

which is finite provided $\kappa > \frac{7}{2}$.

The inequality (14.37) establishes that A_t lies in $\mathcal{K}'$ with probability one. Continuity is proved by a similar argument. The complete details can be found, e.g., in Giacomin *et al.* (2001), Lemma 5.5. □

The path measure for $A_t(x)$, as a probability measure on $C(\mathbb{R}, \mathcal{K}')$, is denoted by $\mathrm{d}\mathsf{P}$. The time-zero field is $A_0(x)$. $A_0(x)$ has the distribution $\mathrm{d}\mathsf{P}^0$ as a probability measure on $\mathcal{K}'$. According to (14.30) $\mathrm{d}\mathsf{P}^0$ is Gaussian with mean zero and covariance

$$\mathbb{E}_{\mathrm{d}\mathsf{P}^0}\big(A_0(f)A_0(g)\big) = \int \mathrm{d}^3k(2\omega)^{-1}\,\widehat{f}^*\cdot Q^\perp\widehat{g}\,. \tag{14.39}$$

As in the case of a single oscillator, there is a natural unitary map U from Fock space $\mathcal{F}$ to $L^2(\mathcal{K}', \mathrm{d}\mathsf{P}^0)$ which is achieved through Wick order. The Wick

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order for operators on $\mathcal{F}$ is defined by moving all creation operators to the left. The Wick-ordered polynomials on $\mathcal{K}'$ are defined through a multilinear extension of the orthogonalization scheme for a single oscillator. Let $X_1, \dots, X_k$ be k random variables. Their Wick order, relative to $\langle\cdot\rangle$, is defined recursively by $:(X_1)^0 \dots (X_k)^0: = 1$, $\langle :(X_1)^{n_1} \dots (X_k)^{n_k}: \rangle = 0$, and $\partial/\partial X_j :(X_1)^{n_1} \dots (X_k)^{n_k}: = n_j :(X_1)^{n_1} \dots (X_j)^{n_j - 1} \dots (X_k)^{n_k}:$. Clearly, for a single degree of freedom, i.e. $\mathcal{K}' = \mathbb{R}$, $\mathrm{d}\mathsf{P}^0 = \sqrt{\omega/\pi}\,\mathrm{e}^{-\omega^2 x^2}\mathrm{d}x$, the Wick order agrees with the construction in (14.15). The unitary map $U : \mathcal{F} \to L^2(\mathcal{K}', \mathrm{d}\mathsf{P}^0)$ is then given by

$$U\Omega = 1\,, \quad U{:}A(f_1) \dots A(f_n){:}\,\Omega = {:}A_0(f_1) \dots A_0(f_n){:}\ . \tag{14.40}$$

Here Ω denotes the Fock vacuum of $\mathcal{F}$. $A(f_j)$ is the quantized vector potential (13.35) smeared by f_j as $A(f_j) = \int \mathrm{d}^3x f_j(x) \cdot A(x)$, whereas to the right stands the Wick order of polynomials as functions on $\mathcal{K}'$. We note that the dynamics is implemented as

$$U\mathrm{e}^{-tH_\mathrm{f}}U^{-1}{:}A_0(f_1) \dots A_0(f_n){:} = {:}A_0(\mathrm{e}^{-\omega t} f_1) \dots A_0(\mathrm{e}^{-\omega t} f_n){:} \tag{14.41}$$

for $t \geq 0$. $UH_\mathrm{f}U^{-1}$, a linear operator acting on $L^2(\mathcal{K}', \mathrm{d}\mathsf{P}^0)$, is referred to as the Schrödinger representation of H_f.

Next we couple the charge and the Maxwell field. According to (14.39) the natural Hilbert space is

$$\mathcal{H}_\mathrm{s} = L^2(\mathbb{R}^3, \mathrm{d}^3x) \otimes L^2(\mathcal{K}', \mathrm{d}\mathsf{P}^0)\,, \tag{14.42}$$

the subscript 's' standing for Schrödinger. The particle Hamiltonian reads $H_\mathrm{p} = -\frac{1}{2}\Delta + V$, with the shorthand $V(q) = e\phi_\mathrm{ex}(q)$, and the field Hamiltonian $UH_\mathrm{f}U^{-1}$ is defined through (14.41). Let us denote by $\mathbb{E}_{\mathrm{d}\mathsf{W}\times\mathrm{d}\mathsf{P}}$ expectation with respect to the path measure $\mathrm{d}\mathsf{W} \times \mathrm{d}\mathsf{P}$, where $\mathrm{d}\mathsf{P}$ is the path measure for the Ornstein–Uhlenbeck process $A_t(x)$ and $\mathrm{d}\mathsf{W}$ the Wiener measure for q_t, i.e. the path measure of Brownian motion with starting distribution d^3x. Let $F, G \in \mathcal{H}_\mathrm{s}$. Then, combining (14.5) and the infinite-dimensional analog of (14.24), we conclude that for the uncoupled system

$$\begin{aligned}\mathbb{E}_{\mathrm{d}\mathsf{W}\times\mathrm{d}\mathsf{P}}\Big(F(q_0, A_0)^* \exp\Big[-\int_0^t \mathrm{d}s\, V(q_s)\Big] G(q_t, A_t)\Big) \\ = \langle 1 \otimes U^{-1}F, \mathrm{e}^{-t(H_\mathrm{p}\otimes 1 + 1 \otimes H_\mathrm{f})} 1 \otimes U^{-1}G\rangle_{\mathcal{H}_\mathrm{s}}\,,\end{aligned} \tag{14.43}$$

$t \geq 0$. In the following, the somewhat pedantic $1\otimes$ will be omitted, in particular U acts on $L^2(\mathbb{R}^3, \mathrm{d}^3x) \otimes \mathcal{F}$ as 1 on the first and as (14.40) on the second factor.

The missing step is to include the minimal coupling to the field through the vector potential. For this purpose we note that in the Hilbert space $L^2(\mathcal{K}', \mathrm{d}\mathsf{P}^0)$ of the Schrödinger representation the transverse vector potential $A(x)$ acts as a

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multiplication operator, compare with (14.40), and in the functional integral the operator $A(x)$ becomes a fluctuating vector potential $A_t(x)$, which is to be inserted in the minimal coupling as $\frac{1}{2}(p - eA_{t\varphi}(q))^2$. Thus one can use (14.7) and (14.8), properly adapted to time-dependent vector potentials respecting the Coulomb gauge $\nabla \cdot A_t = 0$. For later convenience let us reintroduce the mass of the quantum particle, which amounts to replacing $(p - eA_{t\varphi}(q))^2/2$ by $(p - eA_{t\varphi}(q))^2/2m$ and hence taking the Wiener process dW with diffusion coefficient $1/m$ instead of 1, i.e. $\mathbb{E}_0(q_{s\alpha} q_{t\beta}) = m^{-1}\delta_{\alpha\beta} \min(s, t)$. As a result we obtain the functional integral representation for the semigroup e^{-tH}, $t \geq 0$, of the spinless Pauli–Fierz Hamiltonian (13.39) for a single particle as

$$\begin{aligned} &\langle F, U\mathrm{e}^{-tH}U^{-1}G\rangle_{\mathcal{H}_\mathrm{s}} \\ &= \mathbb{E}_{\mathsf{dW}\times\mathsf{dP}}\Big(F(q_0, A_0)^* \exp\Big[-\int_0^t \mathrm{d}s\, V(q_s) - \mathrm{i}e\int_0^t \mathrm{d}q_s \cdot A_{s\varphi}(q_s)\Big] G(q_t, A_t)\Big)\,. \end{aligned} \tag{14.44}$$

Recall that $A_{t\varphi}(q) = \int \mathrm{d}^3x\, \varphi(q - x)A_t(x)$. Equation (14.44) is the basic result of this section. It says that the measure on paths is weighted by the exponential of the classical action. The quadratic terms yield $\mathsf{dW} \times \mathsf{dP}$ and constitute the Gaussian a priori measure of the uncoupled system. The external potential and the minimal coupling to the quantized transverse vector potential are displayed explicitly.

We still have to check that the random variable in the exponential of (14.44) remains finite almost surely. The function $q, s \mapsto A_{s\varphi}(q)$ is (almost surely) continuous in both variables, which makes the stochastic integral well defined. To compute the variance, one notes

$$\mathbb{E}_{\mathsf{dP}}\Big(\Big(\int_0^t \mathrm{d}q_s \cdot A_{s\varphi}(q_s)\Big)^2\Big) = \int_0^t \int_0^t \mathrm{d}q_s \cdot W(q_s - q_{s'}, s - s')\mathrm{d}q_{s'}\,. \tag{14.45}$$

W is the transverse photon propagator,

$$W_{\alpha\beta}(x, t) = \int \mathrm{d}^3k |\widehat{\varphi}(k)|^2 Q^{\perp}_{\alpha\beta}(k) \frac{1}{2\omega} \mathrm{e}^{-\omega|t|}\mathrm{e}^{\mathrm{i}k\cdot x}\,, \tag{14.46}$$

which is bounded by our assumption on $\widehat{\varphi}$. The average of (14.45) with respect to Brownian motion yields

$$\mathbb{E}_{\mathsf{dW}\times\mathsf{dP}}\Big(\delta(q_0)\Big(\int_0^t \mathrm{d}q_s \cdot A_{s\varphi}(q_s)\Big)^2\Big) = t\frac{2}{3m}\int \mathrm{d}^3k |\widehat{\varphi}|^2/2\omega\,, \tag{14.47}$$

since one of the two stochastic differentials points in the future except at the diagonal where $\mathrm{d}q_{t\alpha}\mathrm{d}q_{t\beta} = m^{-1}\delta_{\alpha\beta}\mathrm{d}t$. Thus the action appearing in the exponential of (14.44) has a bounded variance.

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14.2 Integrating out the Maxwell field

We return to the basic formula (14.44) and assume that F, G are of the special form $F(q, A) = G(q, A) = \psi(q)$ with $\psi \geq 0$ and of rapid decrease. The Gaussian integration over $\mathrm{d}\mathsf{P}$ can then be carried out with the result

$$\langle \psi \otimes \Omega, \mathrm{e}^{-tH} \psi \otimes \Omega \rangle_{\mathcal{H}}$$
$$= \mathbb{E}_{\mathrm{d}\mathsf{W}}\Big(\psi(q_0) \exp\Big[-\int_0^t \mathrm{d}s\, V(q_s) - \frac{1}{2}e^2 \int_0^t \int_0^t \mathrm{d}q_s \cdot W(q_s - q_{s'}, s - s')\mathrm{d}q_{s'}\Big]\psi(q_t)\Big). \tag{14.48}$$

Since $\mathrm{d}q_{t\alpha}\mathrm{d}q_{t\beta} = m^{-1}\delta_{\alpha\beta}\mathrm{d}t$ almost surely, we may remove the diagonal cut in the double stochastic integral at the expense of the factor $t(2/3m)\int \mathrm{d}^3k|\widehat{\varphi}|^2/2\omega$. W is the transverse photon propagator (14.46), written more traditionally

$$W(x, t) = \frac{1}{2\pi}\int \mathrm{d}^3k\mathrm{d}k_0|\widehat{\varphi}(k)|^2(k^2 + k_0^2)^{-1}\mathrm{e}^{\mathrm{i}(k\cdot x - k_0 t)}Q^{\perp}(k) \tag{14.49}$$

as a 3×3 matrix. If one removes the ultraviolet cutoff by replacing $\widehat{\varphi}(k)$ by $(2\pi)^{-3/2}$, then (14.49) can be computed explicitly. For our purpose it suffices that qualitatively

$$W(x, t) \cong (x^2 + t^2)^{-1} \tag{14.50}$$

with some modifications due to the transverse projection. Reintroducing $\widehat{\varphi}$ smooths this function at $(x, t) = 0$, but keeps the slow t^{-2} decay. For massive photons, $\omega(k) = (k^2 + m_{\mathrm{ph}}^2)^{1/2}$, this decay would switch to an exponential.

Equation (14.48) looks like the partition function of an equilibrium statistical mechanics system. We regard $\mathrm{d}\mathsf{W}$ as the a priori measure on continuous paths in three-dimensional space. The time interval $[0, t]$ corresponds to the volume. From the point of view of statistical mechanics it is more natural to place it symmetric relative to the origin, i.e. as $[-t, t]$. Configurations are paths q_s, $|s| \leq t$. The factors $\psi(q_{-t})$, $\psi(q_t)$ constrain their end points to be most likely close to the origin. The paths have a Boltzmann weight consisting of two contributions, a single time integral from the external potential and a double time integral induced through the Maxwell field. Our observation suggests that the basic object must be the Gibbs measure for paths q_s, $|s| \leq t$, as given through

$$Z(2t)^{-1}\psi(q_{-t})\psi(q_t)$$
$$\times \exp\Big[-\int_{-t}^t \mathrm{d}s\, V(q_s) - \frac{1}{2}e^2 \int_{-t}^t \int_{-t}^t \mathrm{d}q_s \cdot W(q_s - q_{s'}, s - s')\mathrm{d}q_{s'}\Big]\mathrm{d}\mathsf{W} \tag{14.51}$$

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relative to the Wiener measure $\mathrm{d}\mathsf{W}$ with $Z(2t)$ the normalizing constant (14.48). The average with respect to the probability measure (14.51) is denoted below by $\langle\cdot\rangle_t$ and by $\langle\cdot\rangle_t^0$ for $e = 0$.

The relationship to usual spin systems becomes even more evident upon discretizing time in steps of τ; compare with (14.6). Then, setting $q_{n\tau} = \phi_n$, $\phi_n \in \mathbb{R}^3$, $N\tau = t$, (14.51) becomes

$$\frac{1}{Z}\prod_{n=-N}^{N} \mathrm{d}^3\phi_n \psi(\phi_{-N})\psi(\phi_N) \exp\Big[-\frac{1}{2}\frac{m}{\tau}\sum_{j=-N}^{N-1}(\phi_{j+1}-\phi_j)^2 - \tau\sum_{j=-N}^{N} V(\phi_j) - \frac{1}{2}e^2\sum_{i,j=-N}^{N-1}(\phi_{j+1}-\phi_j)\cdot W(\phi_i-\phi_j, i-j)(\phi_{i+1}-\phi_i)\Big], \tag{14.52}$$

which is the Gibbs measure for a three-component continuous spin system with external potential V, a quadratic nearest-neighbor interaction, and a long-range interaction W. The spin configurations are over a one-dimensional lattice. Alternatively, we may interpret ϕ_j as the position of the j-th monomer of an elastic string (polymer) curling in three-dimensional space. The term $(\phi_{j+1}-\phi_j)^2$ is the usual nearest-neighbor elastic energy. Integrating over the Maxwell field results in an additional long-range elastic interaction between the monomers.

In the picture of an elastic string, cf. figure 14.1, it is natural to distinguish between the case $V = 0$ and a confining potential. Let us first discuss $V = 0$ and for definiteness pin the polymer at both end points, i.e. $q_{-t} = 0 = q_t$. If $e = 0$, then the mean square displacement at the midpoint, given by

$$\langle (q_0)^2\rangle_t^0 = 3t/2m\,, \tag{14.53}$$

reflects the stiffness of the free string. We expect that the interaction renormalizes the stiffness as

$$\langle (q_0)^2\rangle_t \cong 3t/2\sigma \tag{14.54}$$

for large t, which defines the (effective) stiffness σ. The expectation in (14.54) is with respect to the interacting measure (14.51). The long-range interaction should make the polymer stiffer as compared to the free case $e = 0$, which means that the effective stiffness should be increasing with increasing coupling e^2.

To gain a crude idea whether such a picture is at least qualitatively correct we replace $W(q,t)$ by $W(0,t)$ in (14.51). Going back to (14.44) this is equivalent to replacing $A_{s\varphi}(q_s)$ by $A_{s\varphi}(0)$ which is the dipole approximation. By rotation

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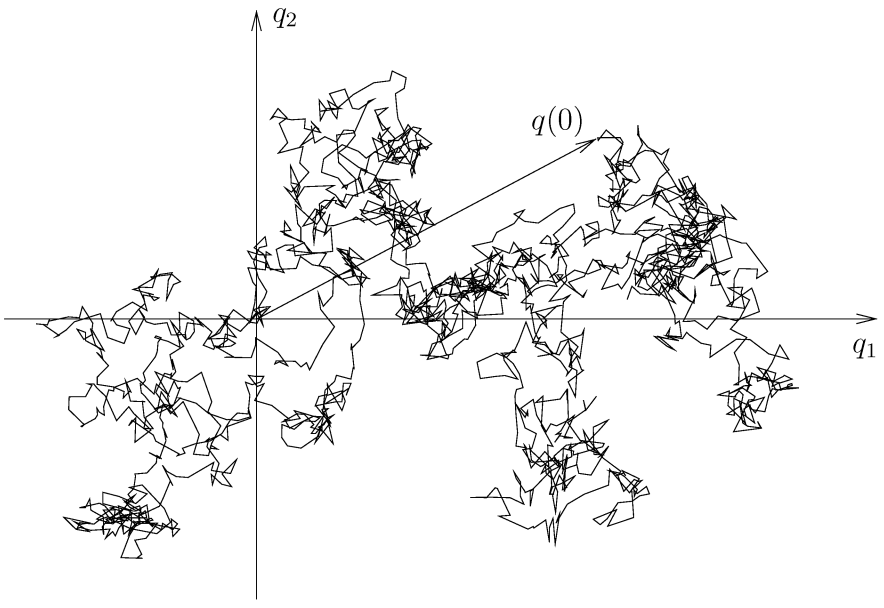

Figure 14.1: Elastic string with end points pinned at the origin.

invariance

$$W_{\alpha\beta}(0,t) = \delta_{\alpha\beta} w(t) \tag{14.55}$$

and we recall that $w(t) \cong 1/t^2$ for large t. In the dipole approximation the Gibbs measure (14.51) is Gaussian and (14.54) can be computed explicitly. One obtains

$$\frac{1}{\sigma} = \int \langle \mathrm{d}q_t \cdot \mathrm{d}q_0 \rangle \,, \tag{14.56}$$

where $\langle \cdot \rangle$ is the infinite-time limit in the dipole approximation, which is Gaussian and has the covariance

$$\langle \mathrm{d}q_t \cdot \mathrm{d}q_0 \rangle = \mathrm{d}t \frac{1}{2\pi} \int \mathrm{d}k_0 (m + e^2 \widehat{w}(k_0))^{-1} \mathrm{e}^{\mathrm{i}k_0 t} \,. \tag{14.57}$$

Therefore,

$$\sigma = m + e^2 \widehat{w}(0) = m + \frac{2}{3} e^2 \int \mathrm{d}^3 k |\widehat{\varphi}|^2 \frac{1}{\omega^2} \,, \tag{14.58}$$

which as anticipated is increasing, in fact linearly in e^2. We remark that if $w(t)$ decays like $1/t$ or even slower, the interaction is so strong that the stiffness is infinite, in the sense that the typical fluctuations of q_0 are no longer of the order $\sqrt{t}$ but grow more slowly with t.

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If one pins only the left end point, $q_{-t} = 0$, one may think of q_t as a random walk with mean square displacement $\langle q_t^2 \rangle = 3D(2t)$ for large t. D is the diffusion coefficient and $D = \sigma^{-1}$ in our units. Thus (14.56), written as

$$D = \int \mathrm{d}t \, \langle \dot{q}_t \cdot \dot{q}_0 \rangle \,, \tag{14.59}$$

is the standard Green–Kubo formula, which expresses D as a time integral over the velocity autocorrelation function. From (14.57) one concludes

$$\langle \dot{q}_t \cdot \dot{q}_0 \rangle = \frac{1}{m}\delta(t) - \frac{1}{2\pi} \int \mathrm{d}k_0 e^2 \widehat{w}(k_0) \big(m(m + e^2 \widehat{w}(k_0))\big)^{-1} \mathrm{e}^{\mathrm{i}k_0 t} \,, \tag{14.60}$$

which is regular except for the δ-function at $t = 0$. The structure (14.60) turns out to be general. For the full Pauli–Fierz Hamiltonian one obtains

$$\langle \dot{q}_t \cdot \dot{q}_0 \rangle = \frac{1}{m}\delta(t) - \langle \psi_0 \,, \frac{1}{m}(P_{\mathrm{f}} + eA_\varphi) \cdot \mathrm{e}^{-|t|(H_0 - E(0))} \frac{1}{m}(P_{\mathrm{f}} + eA_\varphi)\psi_0 \rangle_{\mathcal{F}} \tag{14.61}$$

with a notation which will be explained in section 15.2. Here we just state that with the Definition 15.3 of the effective mass one has the identity

$$\frac{1}{m_{\mathrm{eff}}} = \int \mathrm{d}t \, \langle \dot{q}_t \cdot \dot{q}_0 \rangle = D = \frac{1}{\sigma} \,. \tag{14.62}$$

Thus the stiffness of the polymer in the Euclidean framework equals the effective mass of the charge coupled to the Maxwell field. Note that the regular part of (14.61) is negative, which means that the stiffness is increased as compared to the bare value m. With this background the result (14.58) looks familiar. It is the effective mass of the Abraham model in the nonrelativistic limit; compare with (4.24). The true effective mass of the Pauli–Fierz model has a more complicated dependence on the bare parameters e and m, however.

The second case of interest is a confining potential. For large t the partition function is dominated by the ground state of H, provided it exists at all. In fact, as we will see, ground state expectations can be computed through the limit $t \to \infty$. Thus, as for thermodynamic systems, the infinite-volume limit is of direct physical interest. If the ground state exists, it should be unique and independent of the particular limit procedure. Translated to (14.51) uniqueness means that the limit $t \to \infty$ exists and is independent of the boundary conditions q_{-t} and q_t, at least if they are not allowed to increase too fast. Since t is one-dimensional, such a property will hold, if the energy across the origin is bounded uniformly in the

volume, i.e. if

$$\int_{-\infty}^{0}\int_{0}^{\infty} \mathrm{d}q_s \cdot W(q_s - q_{s'}, s - s')\mathrm{d}q_{s'} \leq c_0\,. \tag{14.63}$$

Because of the stochastic integration, (14.63) cannot be true literally, but only in the sense that there is a small probability for the interaction across the origin to take large values. Stochastic integrals like (14.63) are not easily estimated, but if we set $q_s - q_{s'} = 0$, which is reasonable since V is supposed to be confining, then the interaction energy is

$$\int_{-\infty}^{0} \mathrm{d}s \int_{0}^{\infty} \mathrm{d}s'(q_s \cdot q_{s'})^2 w''(s - s')\,. \tag{14.64}$$

Note that from the stochastic integration we obtain two extra derivatives, which means that $w''(t) \cong t^{-4}$ for large t. If the path q_s does not make too wild excursions, the interaction energy in (14.63) is essentially bounded, which implies uniqueness of the Gibbs measure in (14.51). To have a phase transition for a Gibbs measure in one dimension the interaction has to decay as t^{-2} or slower, which is avoided by two powers in our context.

The statistical mechanics intuition applied to (14.51) suggests that if H_{p} has a ground state $\psi_0(x)$, i.e. if the ground state for the uncoupled system is $\psi_0 \otimes \Omega$, then, as the coupling is turned on, the ground state will persist and remain unique at any coupling strength. For large e^2 fluctuations are suppressed and the ground state must be essentially classical.

14.3 Some applications

(i) Positivity improvement

Let us consider a general measure space $(\mathcal{M}, \mu)$ and the corresponding Hilbert space $L^2(\mathcal{M}, \mu)$ of square integrable functions on $\mathcal{M}$. In addition, we have the semigroup e^{-tH}, $t \geq 0$, acting on $L^2(\mathcal{M}, \mu)$ with $(\mathrm{e}^{-tH})^* = \mathrm{e}^{-tH}$ and $\inf \sigma(H) = 0$, i.e. $\|\mathrm{e}^{-tH}\| = 1$ for $t \geq 0$. We say that e^{-tH} is *positivity preserving*, if for $f \geq 0$ we have $\mathrm{e}^{-tH} f \geq 0$. e^{-tH} is *positivity improving* if $f \geq 0$ implies $\mathrm{e}^{-tH} f > 0$ for $t > 0$. We remark that positivity is not a Hilbert space notion, it depends on the choice of $\mathcal{M}$. Positivity means that, up to normalization, e^{-tH} is a Markov semigroup and some sort of stochastic model is lurking behind. Our interest in the notion of positivity improvement comes from the fact that it implies uniqueness of the ground state. In essence, positivity improvement is the only general criterion available. The reason for uniqueness is simple. Let ψ be an eigenfunction of H with eigenvalue 0. Then by positivity $|\mathrm{e}^{-tH}\psi| \leq \mathrm{e}^{-tH}|\psi|$ and

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thus

$$\langle|\psi|, \mathrm{e}^{-tH}|\psi|\rangle \geq \langle|\psi|, |\mathrm{e}^{-tH}\psi|\rangle \geq \langle\psi, \mathrm{e}^{-tH}\psi\rangle = \langle\psi, \psi\rangle\,. \tag{14.65}$$

As a consequence, since e^{-tH} is a contraction, one has $\mathrm{e}^{-tH}|\psi| = |\psi|$ and, since e^{-tH} is positivity improving, $\mathrm{e}^{-tH}|\psi| = |\psi| > 0$. But then also $\mathrm{e}^{-tH}(|\psi| - \psi) = |\psi| - \psi$. Either $|\psi| - \psi = 0$ in which case $\psi > 0$ or else $|\psi| - \psi > 0$ in which case $\psi < 0$. We conclude that a second eigenvector with eigenvalue zero could not be orthogonal to ψ.

In view of this technique, it is desirable to prove that $U\mathrm{e}^{-tH}U^{-1}$, where H is the spinless Pauli–Fierz Hamiltonian (13.39) with $A_{\mathrm{ex}} = 0$, is positivity improving on $\mathbb{R}^3 \times \mathcal{K}'$ with measure $\mathrm{d}^3x \times \mathrm{d}\mathsf{P}^0$. A look at (14.44) makes positivity an unlikely fact because of the fluctuating phase. The trick to achieve the desired property is to interchange the role of A and $E_\perp$ through the unitary transformation $\mathrm{e}^{-\mathrm{i}\pi N_{\mathrm{f}}/2}$ with

$$N_{\mathrm{f}} = \sum_{\lambda=1,2} \int \mathrm{d}^3k a^*(k, \lambda)a(k, \lambda) \tag{14.66}$$

the total number of photons.

Theorem 14.2 (Positivity improving). *Let $H = \frac{1}{2}(p - eA_\varphi(x))^2 + H_{\mathrm{f}} + V(x)$ be the spinless Pauli–Fierz Hamiltonian with external potential V. Then the semigroup $U\mathrm{e}^{\mathrm{i}\pi N_{\mathrm{f}}/2}\mathrm{e}^{-tH}\mathrm{e}^{-\mathrm{i}\pi N_{\mathrm{f}}/2}U^{-1}$ is positivity improving on $\mathbb{R}^3 \times \mathcal{K}'$ with measure $\mathrm{d}^3x \times \mathrm{d}\mathsf{P}^0$.*

Proof: Hiroshima (2000a).

Corollary 14.3 (Uniqueness of the ground state). *If the spinless Pauli–Fierz Hamiltonian has a ground state, then the ground state is necessarily unique.*

The actual proof of Theorem 14.2 is somewhat technical. But there is a simple heuristic reason to see that it should be correct. We have

$$\mathrm{e}^{\mathrm{i}\pi N_{\mathrm{f}}/2}H\mathrm{e}^{-\mathrm{i}\pi N_{\mathrm{f}}/2} = \frac{1}{2}(p - eE_{\perp\widetilde{\varphi}}(x))^2 + H_{\mathrm{f}} + V(x)\,, \tag{14.67}$$

where the smoothing function φ is replaced by $\widetilde{\varphi}$ with $\widehat{\widetilde{\varphi}} = \widehat{\varphi}/\omega$. We formally discretize the Maxwell field in (14.67) as

$$\frac{1}{2}\left(p - e\sum_j \widetilde{\varphi}(j - x)p_j\right)^2 + \frac{1}{2}\sum_j p_j^2 + \frac{1}{2}\sum_{|i-j|=1}(q_i - q_j)^2 + V(x) \tag{14.68}$$

up to a constant. Here (q_j, p_j) are a canonical pair of position and momentum operators and the sum is over a discrete lattice in position space. We employ the

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usual Feynman–Kac formula. The first two terms define a multidimensional Brownian motion. It has a position-dependent diffusion matrix, which by inspection is strictly positive. Thus the "free" measure is positivity improving, a property which is preserved when adding the potential.

(ii) Diamagnetic inequality

In (14.44) the fluctuating magnetic field appears as a phase, which leads immediately to the *diamagnetic inequality*

$$|\langle F, U\mathrm{e}^{-tH}U^{-1}G\rangle_{\mathcal{H}_\mathrm{s}}| \leq \langle |F|, U\mathrm{e}^{-t(H_\mathrm{p}+H_\mathrm{f})}U^{-1}|G|\rangle_{\mathcal{H}_\mathrm{s}}\,. \tag{14.69}$$

As one application we derive a bound on the electronic charge density in the ground state. We assume the existence of a ground state, $H\psi_\mathrm{g} = E_\mathrm{g}\psi_\mathrm{g}$, with ground state energy E_g. Then the electronic charge density is

$$\rho_\mathrm{g}(x) = \|\psi_\mathrm{g}(x,\cdot)\|^2_{\mathcal{F}} = \sum_{n=0}^{\infty}\sum_{\lambda}\int \mathrm{d}^{3n}k|\psi_{\mathrm{g}n}(x,k_1,\lambda_1,\ldots,k_n,\lambda_n)|^2\,. \tag{14.70}$$

We choose $F = f(x)U\psi_\mathrm{g}$, $f \geq 0$ and bounded, $G = U\psi_\mathrm{g}$. Since $\mathrm{e}^{-tH}\psi_\mathrm{g} = \mathrm{e}^{-tE_\mathrm{g}}\psi_\mathrm{g}$ and since $\mathrm{e}^{-tH_\mathrm{f}}$ is a contraction, one concludes from the diamagnetic inequality that

$$\begin{aligned}\mathrm{e}^{-(t+\tau)E_\mathrm{g}}\int \mathrm{d}^3x f(x)\rho_\mathrm{g}(x) &\leq \langle f\rho_\mathrm{g}^{1/2}, \mathrm{e}^{-(t+\tau)H_\mathrm{p}}\rho_\mathrm{g}^{1/2}\rangle_{L^2}\\ &= \langle \mathrm{e}^{-tH_\mathrm{p}}f\rho_\mathrm{g}^{1/2}, \mathrm{e}^{-\tau H_\mathrm{p}}\rho_\mathrm{g}^{1/2}\rangle_{L^2}\,.\end{aligned} \tag{14.71}$$

From the Feynman–Kac formula (14.5) it follows that $(\mathrm{e}^{-\tau H_\mathrm{p}}\rho_\mathrm{g}^{1/2})(x) \leq c_1$. Using this bound in (14.71) and letting f shrink to a δ-function at x we obtain

$$\rho_\mathrm{g}(x) \leq [c_1\mathrm{e}^{tE_\mathrm{g}}(\mathrm{e}^{-tH_\mathrm{p}}1)(x)]^2 \tag{14.72}$$

with 1 the constant function. Inequality (14.72) is the desired bound on the electronic charge density.

To make this bound explicit we rewrite

$$(\mathrm{e}^{-tH_\mathrm{p}}1)(x) = \mathbb{E}_x\big(\mathrm{e}^{-\int_0^t \mathrm{d}s\,V(q_s)}\big) \tag{14.73}$$

according to (14.5) for the particular choice $\psi(x) = 1$. If the potential has a lower bound as $V(x) \geq c_0 + c_1|x|^\gamma$, $c_1 > 0$, $\gamma > 1$, then for fixed t the weight in (14.73) is dominated by the potential and one has $\rho_\mathrm{g}(x) \leq c\mathrm{e}^{-V(x)}$. On the other hand if $V(x) \to 0$ as $|x| \to \infty$, then the expression in (14.73) tends to 1 as $x \to \infty$. Thus we should optimize in t for fixed x. Very crudely this means minimizing the action $\int_0^t \mathrm{d}s\big(\frac{1}{2}\dot{q}_s^2 + V(q_s)\big)$ for a fixed initial condition $q_0 = x$ and then to optimize in t. In this variation one has to include the contribution from the exponentially growing

factor $\mathrm{e}^{E_{\mathrm{g}}t}$. To have a bound state at all, $V_{\min} = \min_x V(x) < 0$. For sufficiently small e also $V_{\min} - E_{\mathrm{g}} < 0$ and the variational bound decays exponentially in x, i.e. $\rho_{\mathrm{g}}(x) \leq c\mathrm{e}^{-\gamma|x|}$. For larger e one can no longer balance E_{g} and the bound (14.72) becomes vacuous.

The diamagnetic inequality suggests that the decay of the electronic charge density in the ground state does not worsen by the coupling to the Maxwell field. If one imagines, rather crudely, the effective mass of the electron to be increased through the interaction with the field, then the electron density should become even better localized for larger e and point-like as $e \to \infty$.

(iii) Photon expectations

We discovered in section 14.2 that, through integrating over the Maxwell field, one obtains a path integral (functional measure) for the electron paths which has the structure of an equilibrium measure relative to an a priori weight given by the Wiener measure. Here we expand on this observation by computing averages for the photon field in the ground state. Let ψ_0 be the ground state of H_{p} and let us introduce the approximate ground state

$$\psi_T = \mathrm{e}^{-TH}\psi_0 \otimes \Omega / \|\mathrm{e}^{-TH}\psi_0 \otimes \Omega\| \tag{14.74}$$

of H, which is normalized to one and, if the limit does not vanish, converges as $T \to \infty$ to the unique ground state ψ_{g} of H. For observables of the form $f(x)$ the same argument as for (14.48) leads to

$$\begin{aligned} &\langle \psi_T, f(x)\psi_T\rangle_{\mathcal{H}} \\ &\quad = \langle \psi_0 \otimes \Omega, \mathrm{e}^{-2TH}\psi_0 \otimes \Omega\rangle_{\mathcal{H}}^{-1} \langle \psi_0 \otimes \Omega, \mathrm{e}^{-TH} f(x) \mathrm{e}^{-TH}\psi_0 \otimes \Omega\rangle_{\mathcal{H}} \\ &\quad = \mathbb{E}^{\mathrm{G}}_{[-T,T]}\big(f(q_0)\big)\,. \end{aligned} \tag{14.75}$$

The "volume" $[-T, T]$ is arranged symmetrically relative to the origin. $\mathbb{E}^{\mathrm{G}}_{[-T,T]}$ refers to the normalized expectation

$$\mathbb{E}^{\mathrm{G}}_{[-T,T]}\big(\,\circ\,\big) = Z(2T)^{-1}\mathbb{E}_{\mathsf{dW}}\big(\psi_0(q_{-T})\psi_0(q_T)\mathrm{e}^{-\int_{-T}^{T}\mathrm{d}t\,V(q_t)}\mathrm{e}^{-S_{[-T,T]}}\circ\big) \tag{14.76}$$

with the normalizing partition function

$$Z(2T) = \mathbb{E}_{\mathsf{dW}}\Big(\psi_0(q_{-T})\psi_0(q_T)\exp\Big[-\int_{-T}^{T}\mathrm{d}t\,V(q_t) - S_{[-T,T]}\Big]\Big) \tag{14.77}$$

and with the effective action

$$S_{[-T,T]} = \frac{1}{2}e^2\int_{-T}^{T}\int_{-T}^{T}\mathrm{d}q_t \cdot W(q_t - q_s, t-s)\mathrm{d}q_s\,. \tag{14.78}$$

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Clearly, in the infinite-volume limit

$$\lim_{T\to\infty} \langle \psi_T, f(x)\psi_T\rangle_{\mathcal{H}} = \langle \psi_{\mathrm{g}}, f(x)\psi_{\mathrm{g}}\rangle_{\mathcal{H}} = \int \mathrm{d}^3x f(x)\rho_{\mathrm{g}}(x) = \langle f(q_0)\rangle\,. \tag{14.79}$$

Thus the electronic charge density is the distribution of q_0, the position of the path at time $t = 0$, under the infinite-volume Gibbs measure $\langle\cdot\rangle$, i.e. under the probability measure obtained in the limit $T \to \infty$ in (14.76) which we denote by $\langle\cdot\rangle$.

With (14.79) we have opened the first page in the dictionary for the translation from Fock space expectations to Gibbs averages. We plan to expand the dictionary by considering a bounded operator $1 \otimes B$ referring only to the photons and want to compute the expectation

$$\langle \psi_T, 1 \otimes B\psi_T\rangle_{\mathcal{H}}\,, \tag{14.80}$$

which for large T goes over to the ground state expectation $\langle \psi_{\mathrm{g}}, 1 \otimes B\psi_{\mathrm{g}}\rangle_{\mathcal{H}}$.

Using the basic identity (14.44) one can write

$$\begin{aligned}(U\mathrm{e}^{-TH}\psi_0 \otimes \Omega)(q, A)\\ = \mathbb{E}_q\mathbb{E}_A\big(\psi_0(q_t)\exp\Big[-\int_0^T \mathrm{d}t\, V(q_t) - \mathrm{i}e\int_0^T \mathrm{d}q_t\cdot A_{t\varphi}(q_t)\Big]\big)\,,\end{aligned} \tag{14.81}$$

where $\mathbb{E}_A$ refers to the Ornstein–Uhlenbeck process $A_t(x)$ with fixed initial field $A_0 = A$. The Gaussian expectation $\mathbb{E}_A$ can be carried out with the result

$$\begin{aligned}\mathbb{E}_A\big(\mathrm{e}^{-\mathrm{i}e\int_0^T \mathrm{d}q_t\cdot A_{t\varphi}(q_t)}\big) = \mathrm{e}^{-\mathrm{i}eA(f_+)}\exp\Big[-\frac{1}{2}e^2\int_0^T\int_0^T\int \mathrm{d}^3k|\widehat{\varphi}(k)|^2\\ \times \mathrm{d}q_t\cdot Q^{\perp}(k)\mathrm{d}q_s\mathrm{e}^{\mathrm{i}k\cdot(q_t-q_s)}\frac{1}{2\omega}\big(\mathrm{e}^{-\omega|t-s|} - \mathrm{e}^{-\omega t}\mathrm{e}^{-\omega s}\big)\Big]\,,\end{aligned} \tag{14.82}$$

where

$$\widehat{f_+}(k) = \int_0^T \mathrm{d}q_t\widehat{\varphi}\mathrm{e}^{-\mathrm{i}k\cdot q_t}\mathrm{e}^{-\omega t}\,, \tag{14.83}$$

which depends on the path q_t, $0 \le t \le T$.

We have to take the expectation of $1 \otimes B$ with respect to the wave function (14.81), for which it is convenient to regard the adjoint wave function as coming from an integration relative to a Brownian motion running from 0 to $-T$. For this purpose one time-reverses the Brownian motion, which starts then at q_{-T} and ends at q. Upon integrating over $\mathrm{d}q_0$ one obtains the Wiener measure for Brownian

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paths $t \mapsto q_t$, $|t| \leq T$. The expectation $\mathbb{E}_A$ for the adjoint wave function yields an expression as in (14.82) where f_+ is replaced by f_- and

$$\widehat{f}_-(k) = -\int_{-T}^{0} \mathrm{d}q_t \widehat{\varphi} \mathrm{e}^{-\mathrm{i}k\cdot q_t} \mathrm{e}^{-\omega|t|} \tag{14.84}$$

with a minus sign, since $\mathrm{d}q_t$ is odd under time-reversal. The expectation for B is most easily written in Fock space. Then

$$\begin{aligned}
&\langle \psi_0 \otimes \Omega, \mathrm{e}^{-TH}(1 \otimes B)\mathrm{e}^{-TH}\psi_0 \otimes \Omega\rangle_{\mathcal{H}} \\
&\quad = \mathbb{E}_{\mathrm{dW}}\big(\psi_0(q_{-T})\psi_0(q_T)\mathrm{e}^{-\int_{-T}^{T} V(q_t)\mathrm{d}t}\langle \Omega, \mathrm{e}^{\mathrm{i}eA(f_-)} B \mathrm{e}^{-\mathrm{i}eA(f_+)}\Omega\rangle_{\mathcal{F}} \\
&\qquad \times \exp\Big[-\frac{1}{2}e^2\Big(\int_{-T}^{0}\int_{-T}^{0} + \int_{0}^{T}\int_{0}^{T}\Big)\int \mathrm{d}^3k|\widehat{\varphi}|^2 \mathrm{d}q_t \cdot Q^{\perp}\mathrm{d}q_s \mathrm{e}^{\mathrm{i}k\cdot(q_t - q_s)} \\
&\qquad \times \frac{1}{2\omega}\big(\mathrm{e}^{-\omega|t-s|} - \mathrm{e}^{-\omega|t|}\mathrm{e}^{-\omega|s|}\big)\Big]\big).
\end{aligned} \tag{14.85}$$

To make further progress we have to choose particular observables. One example is the generating function for the photon number density in momentum space, i.e.

$$B = \exp\Big[-\sum_{\lambda=1,2}\int \mathrm{d}^3k \mu(k) a^*(k,\lambda)a(k,\lambda)\Big] \tag{14.86}$$

with $\mu \geq 0$. Then

$$\begin{aligned}
\langle \Omega, \mathrm{e}^{\mathrm{i}eA(f_-)} B \mathrm{e}^{-\mathrm{i}eA(f_+)}\Omega\rangle_{\mathcal{F}} &= \exp\Big[-\frac{1}{4}\langle \widehat{f}_-, \omega^{-1/2}Q^{\perp}\omega^{-1/2}\widehat{f}_-\rangle_{\mathfrak{h}} \\
&\quad -\frac{1}{4}\langle \widehat{f}_+, \omega^{-1/2}Q^{\perp}\omega^{-1/2}\widehat{f}_+\rangle_{\mathfrak{h}} - \frac{1}{2}\langle \widehat{f}_-, \omega^{-1/2}Q^{\perp}\mathrm{e}^{-\mu}\omega^{-1/2}\widehat{f}_+\rangle_{\mathfrak{h}}\Big].
\end{aligned} \tag{14.87}$$

Collecting all terms yields

$$\begin{aligned}
&\langle \psi_T, \exp\Big[-\sum_{\lambda=1,2}\int \mathrm{d}^3k \mu(k) a^*(k,\lambda)a(k,\lambda)\Big]\psi_T\rangle_{\mathcal{H}} \\
&\quad = \mathbb{E}^{\mathrm{G}}_{[-T,T]}\big(\exp\Big[-e^2\int_{-T}^{0}\int_{0}^{T}\int \mathrm{d}^3k|\widehat{\varphi}|^2\mathrm{d}q_t \cdot Q^{\perp}\mathrm{d}q_s \mathrm{e}^{\mathrm{i}k\cdot(q_t-q_s)} \\
&\qquad \times \frac{1}{2\omega}\mathrm{e}^{-\omega|t|}\mathrm{e}^{-\omega|s|}\big(\mathrm{e}^{-\mu}-1\big)\Big]\big).
\end{aligned} \tag{14.88}$$

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We differentiate with respect to $\mu(k)$ and obtain the ground state photon number density in momentum space,

$$\sum_{\lambda=1,2} \langle \psi_{\mathrm{g}}, a^*(k,\lambda)a(k,\lambda)\psi_{\mathrm{g}}\rangle_{\mathcal{H}} = -e^2 \frac{1}{2\omega}|\widehat{\varphi}|^2 \int_{-\infty}^{0}\int_{0}^{\infty} \langle \mathrm{d}q_t \cdot Q^{\perp}\mathrm{d}q_s \mathrm{e}^{-\omega|t|}\mathrm{e}^{-\omega|s|}\mathrm{e}^{\mathrm{i}k\cdot(q_t-q_s)}\rangle\,, \quad (14.89)$$

the average with respect to the infinite-volume Gibbs measure. In particular one has the remarkable identity that $\langle \psi_{\mathrm{g}}, N_{\mathrm{f}}\psi_{\mathrm{g}}\rangle_{\mathcal{H}}$ equals the average interaction energy between the right and left half-line in the statistical mechanics system. By the same technique, the photon density in physical space is given by

$$\sum_{\lambda=1,2} \langle \psi_{\mathrm{g}}, a^*(x,\lambda)a(x,\lambda)\psi_{\mathrm{g}}\rangle_{\mathcal{H}} = -e^2 \sum_{\lambda=1,2} \int_{0}^{\infty}\int_{-\infty}^{0} \langle \mathrm{d}q_t \cdot f_\lambda(x-q_t,t)\mathrm{d}q_s \cdot f_\lambda(x-q_s,s)\rangle\,, \quad (14.90)$$

where

$$\widehat{f_\lambda}(k,t) = \widehat{\varphi}\frac{1}{\sqrt{2\omega}}\mathrm{e}^{-\omega|t|}e_\lambda(k)\,. \quad (14.91)$$

Equations (14.89) and (14.90) are only partially useful, since there is too little information on the $\mathrm{d}q_t \cdot Q^{\perp}\mathrm{d}q_s$ correlations, except for the soft photon bound (15.9), (15.14) from which one concludes that

$$-c_0(1+|k|^3) \le \int_{-\infty}^{0}\int_{0}^{\infty} \langle \mathrm{d}q_t \cdot Q^{\perp}\mathrm{d}q_s \mathrm{e}^{-\omega|t|}\mathrm{e}^{-\omega|s|}\mathrm{e}^{\mathrm{i}k\cdot(q_t-q_s)}\rangle \le 0 \quad (14.92)$$

with some positive constant c_0. The interaction energy between right and left is bounded and negative on the average. One would expect also its exponential moments to be bounded. If so, $\langle \psi_{\mathrm{g}}, \mathrm{e}^{-\lambda N_{\mathrm{f}}}\psi_{\mathrm{g}}\rangle_{\mathcal{H}} < \infty$ for all λ by (14.88), which implies that in the ground state the number of photons has a super-exponential decay.

Our method may be applied to other observables of interest. For example the ground state expectation and variance of the vector potential is given by

$$\langle \psi_{\mathrm{g}}, A(x)\psi_{\mathrm{g}}\rangle_{\mathcal{H}} = 0\,, \quad (14.93)$$

$$\langle \psi_{\mathrm{g}}, A(x)^2\psi_{\mathrm{g}}\rangle_{\mathcal{H}} = \langle \Omega, A(x)^2\Omega\rangle_{\mathcal{F}} - \sum_{\lambda=1,2} \Big\langle \Big(\int_{-\infty}^{\infty} \mathrm{d}q_t \cdot f_{\mathrm{A}\lambda}(x-q_t,t)\Big)^2\Big\rangle\,, \quad (14.94)$$

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where

$$\widehat{f}_{\mathrm{A}\lambda} = e_\lambda \widehat{\varphi} \frac{1}{2\omega} \mathrm{e}^{-\omega|t|} \,. \tag{14.95}$$

Similarly for the transverse electric field one has

$$\langle \psi_{\mathrm{g}}, E_\perp(x) \psi_{\mathrm{g}} \rangle_{\mathcal{H}} = 0 \,, \tag{14.96}$$

$$\langle \psi_{\mathrm{g}}, E_\perp(x)^2 \psi_{\mathrm{g}} \rangle_{\mathcal{H}} = \langle \Omega, E_\perp(x)^2 \Omega \rangle_{\mathcal{F}} + \sum_{\lambda=1,2} \Big\langle \Big(\int_{-\infty}^{\infty} \mathrm{d}q_t \cdot f_{\mathrm{E}\lambda}(x - q_t, t) \Big)^2 \Big\rangle \tag{14.97}$$

with $\widehat{f}_{\mathrm{E}\lambda} = \partial_t \widehat{f}_{\mathrm{A}\lambda}$. In fact, the vacuum variances are infinite but become finite when the fields are slightly smeared out. Through the presence of a bound electron the electric field fluctuations are increased whereas the vector field fluctuations are suppressed. Their product remains constant, as required by the uncertainty relation.

We recall that $\langle E \rangle = \langle E_\parallel \rangle + \langle E_\perp \rangle$, the second term being zero by (14.96). From the equations of motion, $\nabla \cdot \langle \psi_{\mathrm{g}}, E(x) \psi_{\mathrm{g}} \rangle_{\mathcal{H}} = e \langle \varphi(x - q_0) \rangle = e\varphi * \rho_{\mathrm{g}}(x)$, ρ_{g} being the electron ground state density of (14.70). Thus, at large distances the average electric field generated by a charge bound in the ground state is the Coulomb field with a strength determined through the bare charge e, from which we conclude that in the Pauli–Fierz model there is *no* charge renormalization.

Notes and references

Section 14.1

Gentle introductions to path integrals are Schulman (1981) and Kleinert (1995) emphasizing statistical mechanics aspects. Roepstorff (1994) treats in detail the quantized Maxwell field. Path integrals with a focus on relativistic quantum field theory are explained in the advanced textbook of Huang (1998). Simon (1979) is a beautiful discussion on the connection between functional integration and the Schrödinger equation. In particular, he explains the Feynman–Kac–Ito formula used in (14.8). Gaussian processes, Wick ordering, and the Schrödinger representation are exhaustively covered in Simon (1974) and Glimm and Jaffe (1987). The functional measure for the Pauli–Fierz Hamiltonian is discussed by Hiroshima (1997b). A standard reference on infinite-dimensional Ornstein–Uhlenbeck processes is Holley and Stroock (1978). In Giacomin *et al.* (2001) martingale-type estimates are explained.

Functional integration has two historical roots which developed apparently completely independently. Feynman (1948), cf. also the textbook by Feynman and

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Hibbs (1965), uses space-time histories to visualize quantum processes. This led to quantum propagators as a "sum over histories". On the other hand, Wiener, Levy, and many other probabilists developed the theory of probability measures on function space (= the space of trajectories) to have a mathematical framework for Brownian motion and diffusion processes. Kac (1950) realized that the two approaches are related through the Wick rotation. The extension to models of quantum fields is achieved by Nelson (1966, 1973). With his insights functional integration became the "secret weapon" and is at the heart of the technical development in constructive quantum field theory through the hands of Glimm, Jaffe, Spencer, Simon, and many, many others. I refer to Glimm and Jaffe (1987).

Section 14.2

The integration over field degrees of freedom is discussed in Feynman and Hibbs (1965) and in Feynman (1948). He tackled a variety of physical problems with this technique. The most widely known is the ground state energy of the polaron (Feynman 1955) for which the analog of (14.48) is estimated through a variational method with a result which covered both the intermediate and strong coupling regime for the first time. To view the effective mass as the stiffness of a polymer is proposed in Spohn (1987). If the Maxwell field is replaced by a scalar field, cf. section 19.2, the double stochastic integral becomes a double Riemann integral, which is much easier to handle. In particular, one obtains reasonable bounds on the effective stiffness with a technique borrowed from Brascamp, Lieb and Lebowitz (1976). To view the path measure (14.51) as a Gibbs measure relative to Brownian motion is stressed in Lőrinczi and Minlos (2001), Betz *et al.* (2002), and Lőrinczi *et al.* (2002a, 2002b).

Section 14.3

Positivity-improving semigroups are treated in Reed and Simon (1978), Chapter XIII.12. For the existence of the ground state we refer to section 15.1. Whenever magnetic fields are involved, the diamagnetic inequality is very helpful; compare for example with Cycon, Froese, Kirsch and Simon (1987). Carmona (1978) uses Brownian motion to estimate ground state properties of $-\Delta + V$. His techniques extend to a charge coupled to a scalar field as discussed in Betz *et al.* (2002). There is also a functional analytic proof of exponential localization, which is patterned after Agmon (1982) in the case of the Schrödinger equation, see Theorem 20.1.