REVIEW ARTICLE

AUXILIARY FIELDS AND THE SIGN PROBLEM

J H SAMSON

Department of Physics, Loughborough University of Technology,

Loughborough, Leicestershire LE11 3TU, England

e-mail: j.h.samson@lut.ac.uk

ABSTRACT

The auxiliary-field quantum Monte Carlo method is reviewed. The Hubbard-Stratonovich transformation converts an interacting Hamiltonian into a non-interacting Hamiltonian in a time-dependent stochastic field, allowing calculation of the resulting functional integral by Monte Carlo methods. The method is presented in a sufficiently general form to be applicable to any Hamiltonian with one- and two-body terms, with special reference to the Heisenberg model and one- and many-band Hubbard models. Many physical correlation functions can be related to correlation functions of the auxiliary field; general results are given here. Issues relating to the choice of auxiliary fields are addressed; operator product identities change the relative dimensionalities of the attractive and repulsive parts of the interaction. Frequently the integrand is not positive-definite, rendering numerical evaluation unstable. If the auxiliary field violates time-reversal invariance, the integrand is complex and this sign problem becomes a phase problem. The origin of this sign or phase is examined from a number of geometrical and other viewpoints and illustrated by simple examples: the phase problem by the spin $\frac{1}{2}$ Heisenberg model, and the sign problem by the attractive SU(N) Hubbard model on a triangular molecule with negative hopping integrals. In the latter case, widely studied in the Jahn Teller literature, the sign is due neither to fermions nor spin, but to frustration. This system is used to illustrate a number of suggested interpretations of the sign problem.

1. Introduction

Much of the richness of condensed matter physics is in the diversity of the ordered low-temperature phases that lie concealed within the interacting-electron Hamiltonian. In studies of these phases, whether magnetic, superconducting or more exotic, it is useful to deal directly with the relevant order parameter field (or auxiliary field coupled to it) as the variables of the system. A natural method is based on *functional* or *path integration:* the Hubbard-Stratonovich transformation (HST)[1] traces out the electronic degrees of freedom, to leave a functional integral over these auxiliary variables. It replaces the Coulomb interaction between electrons by a fluctuating electric field in which non-interacting electrons move. It replaces the exchange interaction in a ferromagnet by a fluctuating molecular field to which the spins respond. This response then determines the effective action or Hamiltonian of the auxiliary field. This is an important tool in areas

ranging from itinerant magnetism[2] to nuclear structure;[3] the functional approach to many-body physics is highlighted by a recent text.[4]

Functional integration has been used for many years as an analytical tool and as a systematic means of obtaining approximations.[5,6] Computing power now available allows Monte Carlo (MC) evaluation of the functional integrals for model Hamiltonians, giving non-perturbative and (in principle) numerically exact results. The task of a MC calculation in *classical* statistical mechanics is to find the expectation value of a function F,

$$\langle F \rangle = \frac{\int_\Gamma F(\mathbf{x})\, w(\mathbf{x}) d\mathbf{x}}{\int_\Gamma w(\mathbf{x}) d\mathbf{x}} , \tag{1}$$

where the weight $w(\mathbf{x})$ would typically be the Boltzmann distribution in classical phase space Γ.[7] Because of the large dimensionality of this space, integration can only be performed by random sampling of points. A uniform random sampling is extremely inefficient for large systems, as most of phase space has exponentially small weight. The Metropolis algorithm therefore generates a sample of points $\mathbf{x}_k$ from the (positive-definite!) distribution $w(\mathbf{x})$, given a means of calculating the ratio $w(\mathbf{x})/w(\mathbf{y})$ for neighboring configurations $\mathbf{x}$ and $\mathbf{y}$.[8] Then the estimator of F is

$$\langle F \rangle = \lim_{n \to \infty} \frac{1}{K} \sum_{k=1}^{K} F(\mathbf{x}_k) . \tag{2}$$

The eigenstates of a *quantum* many-body system cannot usually be sampled directly, and less direct techniques must be used. The term *quantum Monte Carlo* (qMC) covers a large variety of techniques whose common feature is that they determine properties of quantum systems by random sampling.[9,10] This review will concentrate on the auxiliary-field functional integral mentioned above. The configuration space Γ becomes the space of paths $\mathbf{u}(\tau)$ (with imaginary time suitably discretized) and the weight $w[\mathbf{u}]$ the exponential of an action. Such integrals can be evaluated by MC integration *if the action is real* (and the weight therefore positive).

A serious difficulty plaguing qMC calculations is that, in many cases of interest, the weight is not positive. It may become negative and, in the absence of time-reversal invariance, need not be real. The calculation may still proceed if points are sampled from a positive distribution, such as the modulus $|w(\mathbf{x})|$ of the weight, and the sign (or phase) $s(\mathbf{x})=w(\mathbf{x})/|w(\mathbf{x})|$ is absorbed into the integrand. This is feasible if the average sign is close to 1. However, the average sign often tends to zero exponentially with decreasing temperature. At low temperatures the integrand becomes a rapidly oscillating but sparsely sampled function, rendering numerical averages highly unstable and unreliable. This *sign problem* or, in the absence of time-reversal symmetry, *phase problem*, is a major hindrance to low-temperature qMC calculations. This review will consider a number of interpretations of these difficulties, illustrated by simple examples. The problem is commonly believed to be a consequence of Fermi statistics, but it also appears in boson and spin systems and other situations which will be examined here.

1.1. *Hamiltonians*

It is not the aim of this review to discuss the solution of specific model Hamiltonians, but rather to use them to illustrate the method and its difficulties. With this in mind, we shall be concerned with spin Hamiltonians, such as the *Heisenberg model*,

$$H = -\mathbf{B} \cdot \sum_i \mathbf{S}_i - \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j \qquad (3)$$

and fermion Hamiltonians, such as the one-band *Hubbard model*,

$$H = -\sum_{ij} \sum_{s=\uparrow}^{\downarrow} t_{ij} c_{is}^\dagger c_{js} + U \sum_i n_{i\uparrow} n_{i\downarrow}. \qquad (4)$$

This model was originally proposed to describe ferromagnetism in transition metals.[11] (Whether the above Hamiltonian does in fact yield a ferromagnetic state for physically realistic parameters is, three decades later, still a matter of debate.) The Hamiltonian is also being investigated as a candidate for high-temperature superconductivity.

The one-band Hubbard model has $SU(2)$ symmetry: invariance under spin rotations, i.e., unitary transformations of the $\uparrow\downarrow$ basis. We shall also consider certain degenerate Hubbard models, representing many-electron atoms. The simplest such generalization is to allow N "flavors" of electron per site. This leads us to the $SU(N)$ Hubbard model[12,13],

$$H = -\sum_{ij} \sum_{a=1}^{N} t_{ij} c_{ia}^\dagger c_{ja} + \frac{U}{N} \sum_i \left(n_i - \frac{N}{2} \right)^2, \qquad (5)$$

where

$$n_i = \sum_{a=1}^{N} c_{ia}^\dagger c_{ia} \qquad (6)$$

is the total charge on site *i*. The label *a* contains both orbital and spin indices. There is equal repulsion ($U>0$) or attraction ($U<0$) between any pair of electrons on a site. For $N=1$ this is a non-interacting system. For $N=2$ this is the one-band Hubbard model (4) up to a trivial constant and shift in the chemical potential.

We may also wish to retain spin symmetry together with orbital degeneracy, allowing for Hund's rule interactions between different orbitals. This suggests the $SU(N) \times SU(2)$ Hubbard model, [14,15,16]

$$H = -\sum_{ij} \sum_{a=1}^{N} \sum_{s=\uparrow}^{\downarrow} t_{ij} c_{ias}^\dagger c_{jas} + \frac{U}{4N} \sum_i n_i^2 - \frac{I}{N} \sum_i \mathbf{S}_i^2, \qquad (7)$$

where

$$n_i = \sum_{a=1}^{N} \sum_{s=\uparrow}^{\downarrow} c_{ias}^\dagger c_{ias} \quad \text{and} \quad \mathbf{S}_i = \frac{1}{2} \sum_{a=1}^{N} \sum_{st} c_{ias}^\dagger \boldsymbol{\sigma}_{st} c_{iat}. \qquad (8)$$

In this case *a* labels the orbital and *s* the spin. The model was proposed originally to describe the $3d$ transition metals (for which $N=5$).[14] Here the one-band model corresponds to $N=1$ and $I=U/3$. In more realistic models there are three coupling constants, corresponding to an intra-band repulsion, an inter-band exchange interaction and an inter-

band Coulomb interaction.[17] Crystal field splitting and spin-orbit coupling will break the orbital symmetry and introduce further parameters.

All these Hamiltonians can be written in the general form

$$\hat{H} = \hat{H}_1 + \hat{H}_2 \quad,$$
(9)

with one-body term

$$\hat{H}_1 = -\tfrac{1}{2}\left(K_\mu \hat{A}_\mu + K_\mu^* \hat{A}_\mu^\dagger\right)$$
(10)

and two-body interaction

$$\hat{H}_2 = -J_{\mu\nu}\hat{A}_\mu^\dagger \hat{A}_\nu \quad.$$
(11)

The summation convention here is that repeated *Greek* indices μ, ν, … are summed over, while repeated *Roman* indices i, j, … are not. The single-particle operators $\{\hat{A}_\mu, \mu=1\ldots n\}$ form a closed algebra and act on an appropriate Hilbert space, and the coefficients $J_{\mu\nu}$ are the elements of an Hermitian matrix. Hats are used to distinguish operators (and rarely unit vectors) wherever there is danger of confusion. In the Heisenberg model, these operators are spin components $\{S_{ix}, S_{iy}, S_{iz}\}$, with K the magnetic field and J the exchange interaction. In the one-band Hubbard model the operators could be particle-hole operators $\{c_{is}^\dagger c_{jt}\}$, where i labels a Wannier orbital and s the spin eigenvalue, so that the index μ refers to *isjt*. Then K are hopping matrix elements and J, in this case a very sparse matrix, is the on-site repulsion U. The chemical potential may be absorbed into K if necessary. With a suitable free-particle basis, the Hamiltonian is general enough to encompass (for example) the Coulomb interaction, and the Ising, Anderson and Kondo models. In the degenerate Hubbard models (5) and (7) we are expressing the Hamiltonian in terms of the operators

$$\hat{A}_{ij} = \sum_{a=1}^{N} c_{ia}^\dagger c_{ja} \quad\text{and}\quad \hat{A}_{isjt} = \sum_{a=1}^{N} c_{ias}^\dagger c_{jat} \quad\text{respectively.}$$
(12)

The limit $N \to \infty$ is then a classical limit, and $1/N$ expansions are possible.[18,19]

For notational convenience, we shall assume the operators $\hat{A}_\mu$ to be Hermitian, which we can do if necessary by doubling the basis from $\{\hat{A}_\mu\}$ to $\{(\hat{A}_\mu + \hat{A}_\mu^\dagger), i(\hat{A}_\mu - \hat{A}_\mu^\dagger)\}$, and take $\{K_\mu\}$ to be real and $\{J_{\mu\nu}\}$ to be the elements of a real symmetric matrix. Then the one and two body terms become

$$\hat{H}_1 = -K_\mu \hat{A}_\mu$$
(13)

and

$$\hat{H}_2 = -J_{\mu\nu}\hat{A}_\mu \hat{A}_\nu \quad.$$
(14)

1.2. *Overview*

The next section reviews the functional integral approach and discusses the calculation of expectation values. The formalism is expressed in a general way, applicable to any Hamiltonian with one- and two-body terms. In fermion systems, Green functions are

usually calculated directly from the fermion determinant. Some expectation values can be calculated from the auxiliary-field correlations, and the procedure is discussed. There is often a wide choice of auxiliary field representations. Section 3 compares the options, dealing in particular with the choice of auxiliary fields in the Hubbard model. With these preliminaries, Sections 4 and 5 discuss the origin and interpretations of the phase and sign problems. The phase problem can be interpreted geometrically, in terms of the phase acquired by a quantum state as it pursues the auxiliary field. The sign problem is more often encountered, and a number of proposals for its interpretation and circumvention are reviewed. The sign problem is commonly ascribed to Fermi statistics or to spin. Section 6 gives a simple example, a single spinless particle on a triangular molecules. If the ring is frustrated (by enclosing half a flux quantum) a minus sign arises as the particle winds round once. This model illustrates many of the previously discussed interpretations. Finally, brief conclusions and prospects are given in Section 7.

2. Functional integration

A fundamental difference between the classical and quantum statistical mechanics of interacting systems is that, in the latter, one rarely has access to the complete set of eigenstates of the system. Were the operators $\hat{A}_\mu$ to commute, it would be possible to diagonalize the Hamiltonian in terms of their eigenstates, which could be sampled directly in a Monte Carlo simulation. The Ising model is of this form. However, for an arbitrary Hamiltonian H with two-particle interactions, many-body matrix elements of the form $\langle m|e^{-\beta H}|n\rangle$ are much more difficult to calculate than those of the form $\langle m|H|n\rangle$. If H only contains single-particle terms, or β is small, both types of matrix element can be calculated. This is the basis of the Monte Carlo algorithms described below.

2.1. *The Trotter-Suzuki transformation*

A d-dimensional quantum system is related to a (highly anisotropic) $d+1$-dimensional classical one, of width $\beta=1/kT$ in the imaginary time direction. Several Monte Carlo techniques rely on this observation by using the Trotter-Suzuki (TS) formula[20] to divide the imaginary-time interval $0<\tau\leq\beta$ into a large number L of time-slices of width $\Delta\tau = \beta/L$, writing the density operator as the product

$$\exp(-\beta H) = \prod_{l=1}^{L} \exp(-\Delta\tau H) \approx \prod_{l=1}^{L} \left(\prod_{r=1}^{p} \exp(-\Delta\tau H^{(r)}) \right) . \qquad (15)$$

Here the Hamiltonian is written as a sum $\sum_r H^{(r)}$ of a small number p (possibly 1) of terms $H^{(r)}$ which are easier to deal with than the full Hamiltonian. For example, they may be kinetic and potential energy terms, separately diagonalizable but not mutually commuting. The error, expressed as the norm of the difference of the operators on the left and right hand side, is $O(\Delta\tau)$. This follows from the Baker-Campbell-Hausdorff formula[21]

$$\exp(-\Delta\tau H^{(1)})\exp(-\Delta\tau H^{(2)}) = \exp\left(-\Delta\tau(H^{(1)}+H^{(2)}) + \tfrac{1}{2}\Delta\tau^2[H^{(1)}, H^{(2)}] + \cdots\right) . \qquad (16)$$

Higher-order exponential product formulae have been proposed, for example involving fractal decomposition, that promise faster convergence.[22]

The sample space in a quantum Monte Carlo calculation of this density matrix is a set of variables inserted between each factor in Eq. (17). These variables could be

(i)   a complete set of many-body states.
(ii) an overcomplete set of many-body states.
(iii) an auxiliary field which linearizes the interaction term.

The first case leads to the world-line Monte Carlo method,[23] usually in conjunction with a checkerboard decomposition of the Hamiltonian, which will not be further discussed here. The second case corresponds to the *coherent-state functional integral,* corresponding to integration over spin directions in the Heisenberg model. As it is of relevance to later discussions on the phase problem, it is elaborated below. The third case, in which the Hubbard-Stratonovich transformation gives an *auxiliary field functional integral*, is the main topic of this review.

2.2. *Coherent state integration*

The *coherent state functional integral*[24] is used extensively in the field theory of spin models.[25,26] Let us first consider the basis we might use in a finite-dimensional Hilbert space, specifically for a spin s particle. The obvious choice (as used in the world-line MC method) is to choose a quantization direction $\mathbf{n}$ and use the set of $2s+1$ eigenstates $\{|m\rangle, m=-s...s\}$ of $\mathbf{n}\cdot\mathbf{S}$ as a basis. An alternative is to fix the *eigenvalue* to be s and vary the *direction* $\mathbf{n}$ over the unit sphere (called the *Bloch sphere* in this context). This has a number of useful features: the symmetry is preserved, the space is independent of s, which appears only as a parameter in the action, and the machinery of field theory is applicable. Such *coherent states* $|\mathbf{n}\rangle$, obeying $\mathbf{n}\cdot\mathbf{S}|\mathbf{n}\rangle=s|\mathbf{n}\rangle$, form an overcomplete set of states. For $s=\frac{1}{2}$, the coherent states are in one-to-one correspondence with the pure states in the usual spinor basis:

$$|\mathbf{n}\rangle = |\theta, \varphi\rangle = e^{i\psi}\begin{pmatrix} \cos{(\theta/2)}\, e^{-i\phi/2} \\ \sin{(\theta/2)}\, e^{i\phi/2} \end{pmatrix}, \qquad (18)$$

where the phase ψ represents an arbitrary choice of gauge.

To obtain the integral, a resolution of the identity, in the form

$$1 = \frac{2s+1}{4\pi}\int_{-1}^{1} d\cos\theta(\tau) \int_{0}^{2\pi} d\,\varphi(\tau)\, |\mathbf{n}(\tau)\rangle \langle \mathbf{n}(\tau)| \qquad (19)$$

is introduced between each time slice $\tau=l\Delta\tau$ in Eq. (20). The partition function becomes an integral

$$Z = \int \prod_i \prod_{l=1}^{L} \left(\tfrac{2s+1}{4\pi} d\mathbf{n}_{il} \right) \langle \mathbf{n}_{iL} | e^{-\Delta\tau H} | \mathbf{n}_{iL-1} \rangle \langle \mathbf{n}_{iL-1} | \cdots | \mathbf{n}_{i1} \rangle \langle \mathbf{n}_{i1} | e^{-\Delta\tau H} | \mathbf{n}_{iL} \rangle \qquad (21)$$

$$\rightarrow \int \prod_i \mathsf{D}\mathbf{n}_i(\tau)\, e^{-S[\{\mathbf{n}_i(\tau)\}]} \text{ as } L \rightarrow \infty. \qquad (22)$$

The functional integral $\int \mathcal{D}\mathbf{n}_i(\tau)$ is an integral over all closed paths $\mathbf{n}_i(\tau)$, $0 \le \tau \le \beta$, on the unit sphere. The action of the spin-s Heisenberg model (3) is the following functional of the spin directions:

$$S[\{\mathbf{n}_i(\tau)\}] = -is\sum_i S_{\mathrm{WZ}}[\mathbf{n}_i(\tau)] - \int_0^\beta \left(s\mathbf{B}\cdot\sum_i \mathbf{n}_i(\tau) + s^2\sum_{ij} J_{ij}\mathbf{n}_i(\tau)\cdot\mathbf{n}_j(\tau) \right) d\tau. \qquad (23)$$

The action is complex: the *Wess-Zumino* (or *Berry phase* or *Chern-Simons*) term S_{WZ} is the solid angle swept out by the spin in its motion.[25,27] This follows from the phase change $s\Omega$ experienced by the wave function of a spin s particle on rotation around a solid angle Ω. Spin quantization can be derived from interference between such terms, also responsible for topological effects in low-dimensional magnets.

These integrals are in principle susceptible to Monte Carlo evaluation. However, as the physics is in the interference between phases S_{WZ}, there is necessarily a serious phase problem. Random sampling is not the most efficient way of computing Fourier transforms. Takano has investigated the quantum XY model in this way, but was restricted to two time slices, in which case no area is enclosed and the phase vanishes.[28] Vieira and Sacramento, comparing a number of coherent-state representations, find that even for a single spin the phase fluctuations cause difficulties when large numbers of time slices are used.[29] We shall see how similar effects are responsible for the sign problem in the auxiliary-field method.

Similar coherent states can be defined for arbitrary Lie algebras of the operators $\hat{A}_\mu$,[30] leading to functional integrals of the above form,[31] and it is in principle possible to apply the same method to fermion systems. However, the large dimensionality of the space of coherent states makes this less than convenient. A coherent-state formulation of the one-band $U=\infty$ Hubbard model has been formulated, starting from the algebra of the Hubbard operators.[32,33] These coherent states are parametrized by angular variables for the spin, angular variables for the pseudospin (pairing) operators, and Grassmann variables for the fermionic excitations. Such representations do not readily lend themselves to numerical evaluation.

2.3. *Auxiliary-field functional integration*

The method of choice for such correlated-electron systems is the *auxiliary-field functional integral*, giving the *grand canonical* and *projector* Monte Carlo methods. Here a Hubbard-Stratonovich (HST) transformation linearizes the interaction term in each time slice, to obtain a non-interacting system moving in a stochastic *auxiliary field*.[1] The interaction is restored by averaging over the field. One early reference to an auxiliary field, and use of a transformation related to the HST, is in ϕ^4 theory.[34] Another,

relatively straightforward, application is to transform classical spin models (Ising and Heisenberg) to continuous field theories.[35,36] Applications to the Heisenberg and Hubbard models are elaborated in section 3; we shall first outline the general formalism in which there is an interaction between variables $\{x_\mu, \mu = 1 \ldots n\}$ and refer the reader to a number of reviews.[4,37,38]

The transformation relies on an identity such as

$$\exp(M_{\mu\nu} x_\mu x_\nu) = \int \exp(u_\mu x_\mu) \, p(\mathbf{u}) d^n \mathbf{u} \tag{24}$$

to linearize the interaction between the x_μ. The distribution $p(\mathbf{u})$ is often (but not always) a Gaussian

$$p(\mathbf{u}) = [\det(4\pi M)]^{-1/2} \exp\left(-\tfrac{1}{4} M_{\mu\nu}^{-1} u_\mu u_\nu\right). \tag{25}$$

This presupposes that M is a positive-definite matrix (corresponding to an attractive interaction) and that the $\{x_\mu\}$ commute. In that case the Gaussian integral converges, and the result follows from completion of the square. Although the matrices arising here are Hermitian, acting in an n-dimensional (real or complex) vector space V, they are not necessarily positive-definite. We can block-diagonalize the matrix in the three orthogonal subspaces V_+, V_0 and V_-, of dimension n_+, n_0 and n_-, where its eigenvalues are positive, zero and negative respectively:

$$M = \begin{pmatrix} M_+ & 0 & 0 \\ 0 & M_0 & 0 \\ 0 & 0 & M_- \end{pmatrix}, \tag{26}$$

where M_+, $M_0 = 0$, M_- are $n_{+,0,-} \times n_{+,0,-}$ matrices restricted to the respective subspaces, with $V = V_+ \oplus V_0 \oplus V_-$ and $n = n_+ + n_0 + n_-$. We then find a real n_+-component auxiliary field $\mathbf{u} \in V_+$ corresponding to the attractive part of the interaction and an imaginary n_--component auxiliary field $i\mathbf{v}$, $\mathbf{v} \in V_-$, corresponding to the repulsive part:

$$\exp(M_{\mu\nu} x_\mu x_\nu) = \int \exp(u_\mu x_\mu) \, p(\mathbf{u}) d^{n_+} \mathbf{u} \int \exp(i v_\mu x_\mu) \, p(\mathbf{v}) d^{n_-} \mathbf{v}, \tag{27}$$

$$\text{where} \quad p(\mathbf{u}) = [\det(4\pi M_+)]^{-1/2} \exp\left(-\tfrac{1}{4} M_{+\mu\nu}^{-1} u_\mu u_\nu\right)$$
$$\text{and} \quad p(\mathbf{v}) = [\det(-4\pi M_-)]^{-1/2} \exp\left(\tfrac{1}{4} M_{-\mu\nu}^{-1} v_\mu v_\nu\right). \tag{28}$$

In simulations, $\mathbf{u}$ and $\mathbf{v}$ will be real variables (although in analytical work the contour of $\mathbf{v}$ may be deformed to pass through the imaginary saddle point). The number of components of the auxiliary field is the rank $n_+ + n_-$ of the matrix. If the interactions are local, this may be much smaller than the order n of the matrix or the dimensionality of the space of coherent states. For example, in the Hubbard model auxiliary fields couple to spin and charge densities but not to inter-site operators such as $c_{i\uparrow}^\dagger c_{j\uparrow}$, $i \neq j$. The number of variables scales with the number of atoms rather than its square.

We now turn to the quantum case and consider the general Hamiltonian. If the operators do not commute, the identity (29) cannot be applied directly. It is instead applied to the interaction part $\exp(\Delta\tau J_{\mu\nu}\hat{A}_\mu\hat{A}_\nu)$ in each time slice in Eq. (30), so that $M=\Delta\tau J$. For example, with a purely attractive interaction we have

$$\exp\left(J_{\mu\nu}\hat{A}_\mu\hat{A}_\nu\Delta\tau\right) = \left[\det(4\pi J/\Delta\tau)\right]^{-1/2}\int \prod_\mu du_{\mu l}\,\exp\left(-\tfrac{1}{4}J_{\mu\nu}^{-1}u_{\mu l}u_{\nu l}\Delta\tau + u_{\mu l}\hat{A}_\mu\Delta\tau\right) + O(\Delta\tau^2) \tag{31}$$

in the lth time slice. In the limit $\Delta\tau\oslash0$, the operators can be taken to commute. Let us divide the interaction matrix as before into attractive and repulsive subspaces, with matrices J_+ and J_- respectively. The imaginary-time-dependent fields $\mathbf{u}(\tau)=\{u_\mu(\tau)\}$ and $i\mathbf{v}(\tau)=\{iv_\mu(\tau)\}$ coupled to the operators $\hat{\mathbf{A}}$ replace the interaction term; the partition function $z[\mathbf{u},\mathbf{v}]$ of a time-dependent free-particle Hamiltonian $h(\tau)$ is then averaged over the fields to obtain the partition function Z of the interacting system as a functional integral. The grand canonical MC method consists of the numerical evaluation of this integral

$$Z = \frac{\int \mathsf{D}^{n_+}\mathbf{u}(\tau)\,\mathsf{D}^{n_-}\mathbf{v}(\tau)\,\exp(-\beta V_0[\mathbf{u},\mathbf{v}])z[\mathbf{u},\mathbf{v}]}{\int \mathsf{D}^{n_+}\mathbf{u}(\tau)\,\mathsf{D}^{n_-}\mathbf{v}(\tau)\,\exp(-\beta V_0[\mathbf{u},\mathbf{v}])}, \tag{32}$$

where we define

$$\left.\begin{aligned}\mathsf{D}^{n_+}\mathbf{u}(\tau) &\equiv \lim_{L\to\infty}\prod_{l=1}^{L}\prod_{\mu=1}^{n_+} du_{\mu l}\\[2mm]\mathsf{D}^{n_-}\mathbf{v}(\tau) &\equiv \lim_{L\to\infty}\prod_{l=1}^{L}\prod_{\mu=1}^{n_-} dv_{\mu l}\end{aligned}\right\} \tag{33}$$

with $\tau=l\Delta$. The normalization is rather poorly defined, but any infinite factors are removed by the denominator if the limit $L\oslash\infty$ is taken after forming the ratio. The Gaussian weight $\exp(-\beta V_0[\mathbf{u},\mathbf{v}])$ is given by

$$\beta V_0[\mathbf{u},\mathbf{v}] = \tfrac{1}{4}\int_0^\beta \left[J_{+\mu\nu}^{-1} u_\mu(\tau)\,u_\nu(\tau) - J_{-\mu\nu}^{-1} v_\mu(\tau)\,v_\nu(\tau)\right] d\tau \tag{34}$$

and the partition function of the non-interacting system in the auxiliary field is

$$z[\mathbf{u},\mathbf{v}] = \operatorname{Tr}\mathsf{T}\exp\left(-\int_0^\beta \hat{h}_{\mathbf{u}\mathbf{v}}(\tau)\,d\tau\right), \tag{35}$$

where

$$\hat{h}_{\mathbf{u}\mathbf{v}}(\tau) = \left(-K_\mu - u_\mu(\tau) - iv_\mu(\tau)\right)\hat{A}_\mu. \tag{36}$$

We shall call these the *auxiliary partition function* and *auxiliary Hamiltonian* respectively. The subscripts **uv** on h will be used where the fields need to be stated explicitly. As before, **u** (**v**) moves in V_+ (V_-), the n_+ (n_-) dimensional positive (negative) eigenspace of J. The time-ordering symbol $\mathcal{T}$ orders factors with imaginary time increasing from right to left:

$$\mathsf{T} \exp\left(-\int_0^\beta \hat{h}(\tau)\, d\tau\right) = \lim_{\Delta\tau \to 0} e^{-\Delta\tau \hat{h}(\beta)} \cdots e^{-\Delta\tau \hat{h}(2\Delta\tau)} e^{-\Delta\tau \hat{h}(\Delta\tau)}. \tag{37}$$

The notation $\hat{h}(\tau)$ indicates that $\hat{h}$ has explicit τ dependence through the auxiliary fields; the subscript τ in $\hat{A}_{\mu\tau}$ is a label for time-ordering purposes. Time ordering is required, as $\hat{h}(\tau)$ and $\hat{h}(\tau')$ do not commute for $\tau \neq \tau'$.

The functional integral can be viewed in various ways. Firstly, the partition function is that of an auxiliary field coupled to the system, divided by that of the free auxiliary field. Secondly, in diagrammatic language, $z[\mathbf{u},\mathbf{v}]$ is a sum of all bubble diagrams in Fig. 1, where the full line corresponds to the propagator of $\hat{A}$ in the non-interacting Hamiltonian $-K_\mu \hat{A}_\mu$ and the dashed line corresponds to the auxiliary fields. The Gaussian averaging then reconnects the ends of the dashed lines to recover the interacting system.
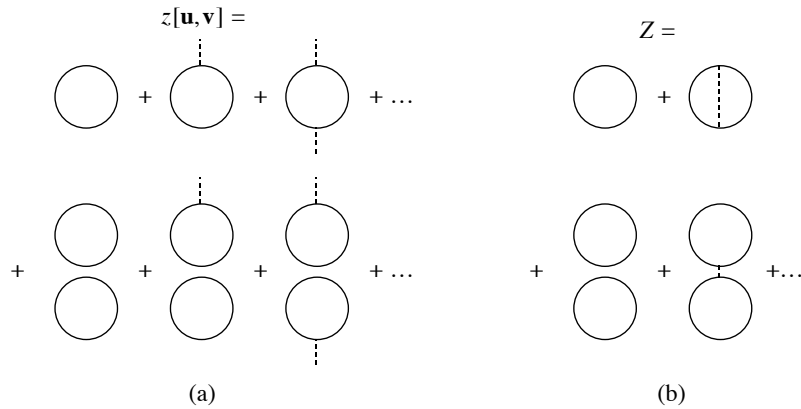

Fig. 1. Diagrammatic expansion of (a) the partition function of the non-interacting system in the auxiliary field and (b) the interacting system recovered after averaging.

The HST has transformed a quantum system into a $d+1$-dimensional classical system. Hertz has carried out a renormalization-group study of phase transitions in quantum systems.[39] At finite temperature, the width in the time direction is finite; at a finite-temperature phase transition there is a crossover to the classical d-dimensional fixed point once the correlation length exceeds this width.

In addition to finite temperature properties, auxiliary-field qMC can give information on ground state properties.[40,41] The *projector qMC method* starts with a trial wave function $|\Psi_\mathrm{T}\rangle$, assumed not to be orthogonal to the true ground state $|\Psi_0\rangle$. The ground state is then

$$|\Psi_0\rangle = \lim_{\beta \to \infty} \frac{e^{-\beta \hat{H}} |\Psi_T\rangle}{\sqrt{\langle \Psi_T | e^{-2\beta \hat{H}} | \Psi_T \rangle}} . \tag{38}$$

The HST is then used to evaluate the density operator in the numerator. In this case, rather than being sampled over all paths $(\mathbf{u}(\tau), \mathbf{v}(\tau))$, the wave function is propagated in imaginary time $0 \leq \tau < \beta$. Since the evolution operator is not unitary, in fermion systems it is necessary to re-orthogonalize the basis states for the Slater determinants at intervals to avoid collapse onto a Bose-condensed state.

We shall normally be assuming a continuum limit in the time direction, while remembering that the auxiliary fields are integration variables with no intrinsic dynamics within each time slice and not continuous functions of time. Discretization of the functional integral is equivalent to restricting the integration in the space of paths $\mathbf{u}(\tau)$ to piecewise-constant paths

$$\mathbf{u}(\tau) = \mathbf{u}_l \text{ where } (l{-}1)\Delta\tau \leq \tau < l\Delta\tau. \tag{39}$$

In a fermion system, $h(\tau)$ describes electrons in a random field and is itself hard to diagonalize. In that case, the TS formula is normally used to split the kinetic and potential energy in each time slice $\tau{=}l\Delta\tau$:

$$\exp\left(-\Delta\tau \hat{h}_{\mathbf{uv}}(\tau)\right) = \exp\left(\Delta\tau (u_{\mu l}{+}iv_{\mu l}) \hat{A}_\mu\right) \exp\left(\Delta\tau K_\mu \hat{A}_\mu\right) + O(\Delta\tau^2) . \tag{40}$$

This is equivalent to restricting integration to paths

$$\mathbf{u}(\tau) = \sum_{l=1}^{L} \mathbf{u}_l \delta(\tau{-}l\Delta\tau) \tag{41}$$

so that the electrons disperse freely, according to their kinetic energy, between random potential energy kicks at regular intervals $\Delta\tau$.

A further restriction of the integration, to time-independent paths, gives the *static approximation* (SA),[42,43] widely used in the context of itinerant magnetism. Here the auxiliary field is constrained to be time-independent, and the functional integral becomes an ordinary integral over the u_μ and v_μ:

$$Z_{SA} = \frac{\int d^{n_+}\mathbf{u}\, d^{n_-}\mathbf{v}\, \exp(-\beta V_0(\mathbf{u},\mathbf{v})) z(\mathbf{u},\mathbf{v})}{\int d^{n_+}\mathbf{u}\, d^{n_-}\mathbf{v}\, \exp(-\beta V_0(\mathbf{u},\mathbf{v}))} , \tag{42}$$

where

$$V_0(\mathbf{u},\mathbf{v}) = \tfrac{1}{4}\left[J_{+\mu\nu}^{-1} u_\mu u_\nu - J_{-\mu\nu}^{-1} v_\mu v_\nu \right] \tag{43}$$

and

$$z(\mathbf{u},\mathbf{v}) = \text{Tr} \exp(-\beta h), \tag{44}$$

where

$$h = \left(-K_\mu - u_\mu - iv_\mu\right) \hat{A}_\mu . \tag{45}$$

This reduces the TS decomposition of Eq. (15) to a single time slice ($L=1$, $p=1$). The end result is a complete diagrammatic summation as in Fig. 1 but with interaction lines restricted to zero Matsubara frequencies.

This reduces the system to the classical statistical mechanics of an effective Hamiltonian $V_{SA}(\mathbf{u},\mathbf{v})=V_0(\mathbf{u},\mathbf{v})-kT\ln z(\mathbf{u},\mathbf{v})$. For the Heisenberg model $z(\mathbf{u},\mathbf{v})$ is simply the partition function of independent spins in magnetic fields $\mathbf{B}+\mathbf{u}_i$, and the effective Hamiltonian is easy to calculate. For the Hubbard model it can be calculated by electronic structure techniques, using fitted tight-binding parameters for iron.[44] This then gives effective exchange interactions between the auxiliary fields on different sites (which will in general include many-atom terms), which can be treated by a classical MC simulation.[45] Others consider the random auxiliary field as a disordered alloy and apply the coherent potential approximation.[46,47,48]

A justification of the SA is the separation of time scales: transverse fluctuations of magnetization are typically much slower than electron hopping times. A number of difficulties do arise. Firstly, the ground state energy in the SA is the minimum of $V_{SA}(\mathbf{u},\mathbf{v})$. This minimum corresponds to a variational ground state of the original Hamiltonian in the space of uncorrelated states that (depending on the choice of auxiliary fields) may be the Hartree-Fock state. The SA is however correct in the high-temperature limit. One consequence is an underestimate of the heat capacity, which can even become negative.[49,50] A second difficulty is that the transformation to a static disordered alloy has destroyed the normal Fermi liquid behavior.[51] Thirdly, as the effective Hamiltonian is classical the high-frequency excitations are overestimated. One can improve on the SA either in the time domain, by adding time slices, or in the frequency domain, by including some non-zero Matsubara frequencies.[52] The recovery of the correct physical properties with increasing number of time slices or frequencies does not seem to have been widely studied.

2.4. *Expectation values and correlation functions*

There are two ways of extracting expectation values from the simulation: from the auxiliary Hamiltonian directly or from the auxiliary field distribution. The former method can be used for any expectation value, while the latter is restricted to products of operators appearing in the interaction term. The methods are demonstrated for a general Hamiltonian.

We first consider the direct method. To evaluate the thermal expectation value of an operator $\hat{F}$ (in general, involving time-ordered products of operators at different times),

$$\langle \hat{F} \rangle \equiv \frac{\mathrm{Tr}\,\mathsf{T}\,\{\hat{F}(\tau_1, \tau_2, \cdots)\exp(-\beta\hat{H})\}}{\mathrm{Tr}\,\mathsf{T}\,\exp(-\beta\hat{H})} , \tag{46}$$

we first convert it into the corresponding functional of the auxiliary fields, $F[\mathbf{u}, \mathbf{v}]$, and take the functional average:

$$\left\langle \hat{F} \right\rangle = \overline{F[\mathbf{u},\mathbf{v}]} \equiv \frac{\int D^{n_+}\mathbf{u}(\tau)\, D^{n_-}\mathbf{v}(\tau)\, F[\mathbf{u},\mathbf{v}]\, w[\mathbf{u},\mathbf{v}]}{\int D^{n_+}\mathbf{u}(\tau)\, D^{n_-}\mathbf{v}(\tau)\, w[\mathbf{u},\mathbf{v}]} \,, \tag{47}$$

where the overbar denotes functional averaging over the auxiliary field with weight

$$w[\mathbf{u},\mathbf{v}] = \exp(-\beta V_0[\mathbf{u},\mathbf{v}])z[\mathbf{u},\mathbf{v}] \tag{48}$$

and the functional $F[\mathbf{u},\mathbf{v}]$, the expectation value of $\hat{F}$ in the time-dependent fields, is

$$F[\mathbf{u},\mathbf{v}] = z[\mathbf{u},\mathbf{v}]^{-1} \, \mathrm{Tr}\, \mathsf{T} \left\{ \hat{F} \exp\left(-\int_0^\beta \hat{h}_{\mathbf{uv}}(\tau)\, d\tau\right) \right\}. \tag{49}$$

It is then in a form that allows MC averaging by importance sampling over the auxiliary field with weight w (if the weight is positive).

There are simple expressions for the expectation values in fermion systems. In that case the above expectation value (50) is taken with respect to a single-particle Hamiltonian, which can be written in the matrix form

$$\hat{h}(\tau) = \sum_{ij} h_{ij}(\tau)c_{i\tau}^\dagger c_{\tau j}, \tag{51}$$

where the spin indices have been suppressed for notational convenience and the chemical potential has been absorbed into the Hamiltonian. For a time-*independent* single-particle Hamiltonian

$$\hat{H} = \sum_{ij} H_{ij}c_i^\dagger c_j \tag{52}$$

where the matrix H has eigenvalues E_k, the trace is simple:

$$\mathrm{Tr}\, \exp(-\beta \hat{H}) = \prod_k \left(1+\exp(-\beta E_k)\right) = \det\left(1+\exp(-\beta H)\right). \tag{53}$$

The left hand side is the trace of the density *operator* over a 2^m-dimensional Fock space of the electrons, while the right hand side is the determinant of an $m \infty m$ *matrix*. The same identity applies to the time-dependent Hamiltonian:[53,54]

$$\mathrm{Tr}\, \mathsf{T} \exp\left(-\int_0^\beta \hat{h}(\tau)\, d\tau\right) = \det\left(1+\mathsf{T}\exp\left(-\int_0^\beta h(\tau)\, d\tau\right)\right), \tag{54}$$

where we shall use the same time-ordering symbol to order matrices chronologically in the same way as operators. Green functions are similarly given by the appropriate elements of the inverse, for example

$$\left\langle c_i c_j^\dagger \right\rangle = \overline{\left[1+\mathsf{T}\exp\left(-\int_0^\beta h(\tau)\, d\tau\right)\right]_{ij}^{-1}}, \tag{55}$$

with similar expressions for the time-dependent Green functions.[54] Since electrons in the auxiliary Hamiltonian (56) are uncorrelated, one can use the machinery of Wick's theo-

rem to contract higher-order Green functions before taking the functional average. Averaging over the auxiliary field then reintroduces the correlations. This therefore allows calculation of correlation functions and response functions in a fermion system.

The other way of extracting correlation functions requires knowledge only of the auxiliary field and is not restricted to fermion or boson systems. The method relies on a close relation between correlation functions of the auxiliary field and those of the operators.[55,56] This can be seen by adding an external field $\mathbf{z}(\tau)=\mathbf{x}(\tau)+\mathbf{y}(\tau)$, where $\mathbf{x}(\tau)\in V_+$ and $\mathbf{y}(\tau)\in V_-$, to the Hamiltonian and taking the partition function as a generating functional for the correlations:

$$\hat{H}'(\tau) = \hat{H} - z_\mu(\tau)\,\hat{A}_{\mu\tau}\,. \tag{57}$$

The partition function of the Hamiltonian $\hat{H}'$ is

$$Z[\mathbf{z}] = e^{-\beta\Omega[\mathbf{z}]} = Z[\mathbf{0}]\left\langle \mathrm{T}\,\exp\left(\int_0^\beta d\tau\,z_\mu(\tau)\,\hat{A}_\mu(\tau)\right)\right\rangle \tag{58}$$

where the *explicit* time dependence of the operators in the above equation is

$$\hat{A}_\mu(\tau) = e^{\tau\hat{H}}\,\hat{A}_{\mu\tau}e^{-\tau\hat{H}}. \tag{59}$$

The cumulant expansion[57] of the grand potential Ω in $\mathbf{z}$ gives the series

$$\Omega[\mathbf{z}] = \Omega[\mathbf{0}] - kT\int_0^\beta d\tau\langle\hat{A}_\mu\rangle z_\mu(\tau)$$
$$- \frac{1}{2}kT\int_0^\beta d\tau_1\int_0^\beta d\tau_2\langle\mathrm{T}\{\hat{A}_\mu(\tau_1)\,\hat{A}_\nu(\tau_2)\}\rangle_c z_\mu(\tau_1)z_\nu(\tau_2) + \cdots \tag{60}$$

where the second-order connected correlation function (or cumulant) $\langle\cdots\rangle_c$ is defined by

$$\langle A\hat{B}\rangle_c = \langle A\hat{B}\rangle - \langle A\rangle\langle B\rangle. \tag{61}$$

Functional derivatives with respect to $\mathbf{x}$ and $\mathbf{y}$ therefore yield correlation functions of the $\hat{\mathbf{A}}$ in the usual way. We can produce a similar expansion in the functional integral formulation by

$$Z[\mathbf{z}] = \frac{\int D^{n_+}\mathbf{u}(\tau)\,D^{n_-}\mathbf{v}(\tau)\,\exp(-\beta V_0[\mathbf{u},\mathbf{v}])\ \mathrm{Tr}\,\mathrm{T}\exp\left(\int_0^\beta (K_\mu+u'_\mu(\tau)+iv'_\mu(\tau))\,\hat{A}_{\mu\tau}\,d\tau\right)}{\int D^{n_+}\mathbf{u}(\tau)\,D^{n_-}\mathbf{v}(\tau)\,\exp(-\beta V_0[\mathbf{u},\mathbf{v}])} \tag{62}$$

where

$$u'_\mu(\tau) = (u_\mu(\tau)+x_\mu(\tau)) \tag{63}$$

and

$$v'_\mu(\tau) = (v_\mu(\tau)-i\,y_\mu(\tau))\,. \tag{64}$$

We now change the variables of integration in the numerator to $\mathbf{u}'(\tau)$ and $\mathbf{v}'(\tau)$. This is allowed, as the space of integration is the space of paths in V_+ and V_- respectively; there is simply a shift in origin by $\mathbf{x}(\tau)$ and $-i\mathbf{y}(\tau)$ respectively.[58] From Eq. (65) we get

$$\beta V_0[\mathbf{u},\mathbf{v}] = \beta V_0[\mathbf{u}',\mathbf{v}']$$
$$+\tfrac{1}{4}\int_0^\beta \left[J_{+\mu\nu}^{-1}\left(-2u_\mu'(\tau)\,x_\nu(\tau)+x_\mu(\tau)\,x_\nu(\tau)\right) + J_{-\mu\nu}^{-1}\left(-2iv_\mu'(\tau)\,y_\nu(\tau)+y_\mu(\tau)\,y_\nu(\tau)\right) \right]d\tau \,. \quad (66)$$

This gives an expression for the partition function as a functional average (with $\mathbf{u}'$ and $\mathbf{v}'$ now relabeled $\mathbf{u}$ and $\mathbf{v}$)

$$Z[\mathbf{z}] = Z[\mathbf{0}]\,\overline{\exp\left(\tfrac{1}{2}\int_0^\beta \left[J_{+\mu\nu}^{-1}\,u_\mu(\tau)\,x_\nu(\tau)+iJ_{-\mu\nu}^{-1}\,v_\mu(\tau)\,y_\nu(\tau)\right]d\tau\right)}$$
$$\times \exp\left(-\tfrac{1}{4}\int_0^\beta \left[J_{+\mu\nu}^{-1}\,x_\mu(\tau)\,x_\nu(\tau) + J_{-\mu\nu}^{-1}\,y_\mu(\tau)\,y_\nu(\tau)\right]d\tau\right) \,. \quad (67)$$

The grand potential can be expanded in powers of $\mathbf{z}$:

$$\Omega[\mathbf{z}] = \Omega[\mathbf{0}] - kT\tfrac{1}{2}\int_0^\beta d\tau\left[J_{+\mu\nu}^{-1}\,\overline{u_\mu}+iJ_{-\mu\nu}^{-1}\,\overline{v_\mu}\right]z_\nu(\tau)$$
$$-\tfrac{1}{8}kT\int_0^\beta d\tau_1\int_0^\beta d\tau_2\left[J_{+\mu\xi}^{-1}J_{+\nu\pi}^{-1}\,\overline{u_\xi(\tau_1)u_\pi(\tau_2)}^c - J_{-\mu\xi}^{-1}J_{-\nu\pi}^{-1}\,\overline{v_\xi(\tau_1)v_\pi(\tau_2)}^c\right]z_\mu(\tau_1)z_\nu(\tau_2)$$
$$+\tfrac{1}{4}kT\int_0^\beta d\tau\left[J_{+\mu\nu}^{-1} + J_{-\mu\nu}^{-1}\right]z_\mu(\tau)z_\nu(\tau) + \cdots \qquad\qquad . \quad (68)$$

Comparing the expansions (69) and (70) gives us the relation we are seeking between operator and auxiliary field correlation functions. If we write the projection of the operators $\hat{A}_\mu$ onto the subspaces $V_\pm$ as $\hat{A}_{\pm\mu}$, we get a relation for the expectation values of the operators

$$\left.\begin{aligned}
\langle \hat{A}_{+\mu}\rangle &= \tfrac{1}{2}J_{+\mu\nu}^{-1}\,\overline{u_\mu} \\
\langle \hat{A}_{-\mu}\rangle &= \tfrac{1}{2}iJ_{-\mu\nu}^{-1}\,\overline{v_\mu}
\end{aligned}\right\} \qquad\qquad . \quad (71)$$

(It should be pointed out here that, although the auxiliary field $\mathbf{v}$ is real, its average is imaginary when taken with respect to the complex weight $w[\mathbf{u},\mathbf{v}]$. The expectation value of the operator $\hat{A}_{-\mu}$ is therefore real.)

Correlation functions are calculated similarly:

$$\left.\begin{aligned}
\langle T\{\hat{A}_{+\mu}(\tau_1)\,\hat{A}_{+\nu}(\tau_2)\}\rangle_c &= \tfrac{1}{4}J_{+\mu\xi}^{-1}J_{+\nu\pi}^{-1}\,\overline{u_\xi(\tau_1)u_\pi(\tau_2)}^c - \tfrac{1}{2}J_{+\mu\nu}^{-1}\delta(\tau_1-\tau_2) \\
\langle T\{\hat{A}_{-\mu}(\tau_1)\,\hat{A}_{-\nu}(\tau_2)\}\rangle_c &= -\tfrac{1}{4}J_{-\mu\xi}^{-1}J_{-\nu\pi}^{-1}\,\overline{v_\xi(\tau_1)v_\pi(\tau_2)}^c - \tfrac{1}{2}J_{-\mu\nu}^{-1}\delta(\tau_1-\tau_2)
\end{aligned}\right\} \quad (72)$$

with higher order cumulants equal (up to a linear transformation J):

$$\left.\begin{aligned}\left\langle\mathsf{T}\left\{\hat{A}_{+\mu}(\tau_1)\cdots\hat{A}_{+\omega}(\tau_r)\right\}\right\rangle_c &= 2^{-r}J_{+\mu\alpha}^{-1}\cdots J_{+\omega\lambda}^{-1}\overline{u_\alpha(\tau_1)\cdots u_\lambda(\tau_2)}^{\,c}\\[4pt]\left\langle\mathsf{T}\left\{\hat{A}_{\mu}(\tau_1)\cdots\hat{A}_{\omega}(\tau_r)\right\}\right\rangle_c &= (-2i)^{-r}J_{-\mu\alpha}^{-1}\cdots J_{-\omega\lambda}^{-1}\overline{v_\alpha(\tau_1)\cdots v_\lambda(\tau_2)}^{\,c}\end{aligned}\right\}\qquad (r>2). \tag{73}$$

Thus in the Hubbard model, discussed in detail in Section 3.3, we can calculate spin-spin correlation functions (corresponding to the positive subspace) and charge-charge correlation functions (corresponding to the negative subspace). Other quantities, such as inter-site Green functions, that cannot be expressed in terms of spin and charge densities involve the zero subspace and cannot be derived from the auxiliary field in this way. The first method can of course still be used here.

2.5. Non-positivity

The auxiliary-field quantum Monte Carlo method involves a numerical evaluation of these expectation values. This is straightforward if w is positive-definite: the Metropolis algorithm allows sampling of paths according to the distribution w and (if the process is ergodic) the expectation value is given by

$$\langle\hat{F}\rangle = \lim_{K\to\infty}\frac{1}{K}\sum_{k=1}^{K}F[\mathbf{u}_k,\mathbf{v}_k]\;. \tag{74}$$

Here $[\mathbf{u}_k,\mathbf{v}_k]$ represents the kth path, and the paths are sampled from the distribution w.

In a classical simulation, w is typically a Boltzmann distribution and manifestly positive. In a quantum simulation, w is *not* in general positive-definite. First noted in studies of fermions coupled to a boson field,[53] it also appears, for example, in spin[10] and Jahn-Teller[59] systems. There are two such cases: if w can be negative, we talk of a *sign problem*, and, if it is complex, we shall talk of a *phase problem*. The latter case applies if the auxiliary field breaks time-reversal invariance, for example for the $\mathbf{v}$ field arising from a repulsive interaction or a $\mathbf{u}$ field coupled to a three-component spin. In each case the auxiliary Hamiltonian is complex. However, for each path $\mathbf{u}(\tau)$, $\mathbf{v}(\tau)$ there is a conjugate path

$$\left.\begin{aligned}\tilde{\mathbf{u}}(\tau) &= !\mathbf{u}(\beta-\tau)\\\tilde{\mathbf{v}}(\tau) &= -\mathbf{v}(\beta-\tau)\end{aligned}\right\}. \tag{75}$$

The weight of this conjugate path is the complex conjugate of that of the original path:

$$\begin{aligned}w[\tilde{\mathbf{u}},\tilde{\mathbf{v}}] &= \mathrm{Tr}\,\mathsf{T}\exp\int_0^\beta\left(K_\mu+u_\mu(\beta-\tau)-iv_\mu(\beta-\tau)\right)\hat{A}_{\mu\tau}d\tau\,\exp\!\left(-\beta V_0[\tilde{\mathbf{u}},\tilde{\mathbf{v}}]\right)\\[4pt]&= \mathrm{Tr}\left(\mathsf{T}\exp\int_0^\beta\left(K_\mu+u_\mu(\tau)+iv_\mu(\tau)\right)\hat{A}_{\mu\tau}d\tau\right)^\dagger\exp\!\left(-\beta V_0[\mathbf{u},\mathbf{v}]\right)\\[4pt]&= w[\mathbf{u},\mathbf{v}]^*\;.\end{aligned} \tag{76}$$

Since both a path and its conjugate appear in the integration, if a real quantity is to be averaged only the real part of w is needed.

Non-positivity is not a formal difficulty in principle; indeed, Feynman has argued that one should not be afraid of using negative probabilities as intermediate results.[60] Why then is it a sign *problem*? The difficulty is in evaluation of the integral. It is still evaluated by importance sampling from a positive-definite weight, usually $|w|$. The sign (or phase factor) $s=w/|w|$ is absorbed into the integrand. Expectation values are

$$\langle \hat{F} \rangle = \frac{\int D^{n_+}\mathbf{u}(\tau)\, D^{n_-}\mathbf{v}(\tau)\, F[\mathbf{u},\mathbf{v}]\, s[\mathbf{u},\mathbf{v}]\, |w[\mathbf{u},\mathbf{v}]|}{\int D^{n_+}\mathbf{u}(\tau)\, D^{n_-}\mathbf{v}(\tau)\, s[\mathbf{u},\mathbf{v}]\, |w[\mathbf{u},\mathbf{v}]|} = \lim_{K\to\infty} \frac{\frac{1}{K}\sum_{k=1}^{K} F[\mathbf{u}_k,\mathbf{v}_k] s[\mathbf{u}_k,\mathbf{v}_k]}{\frac{1}{K}\sum_{k=1}^{K} s[\mathbf{u}_k,\mathbf{v}_k]}, \tag{77}$$

where the points are sampled from the positive distribution $|w|$. (For complex weights one can also sample from the distribution $|\mathrm{Re}\,w|$.) The average sign (in the denominator) typically vanishes exponentially in the low temperature limit.[61] At low temperatures, the statistics will be overwhelmed by noise.

There are other difficulties at low temperatures, related to the ill-conditioned nature of the fermion matrix, which will not be discussed here.[62] We shall return to the phase and sign problems in Sections 4 and 5, after discussing some more concrete examples of the formalism.

3. Examples

3.1. *Coulomb interaction*

Before tackling quantum systems, let us consider how auxiliary fields might be used in an electrostatic system, where they have a clearer physical interpretation. The classical non-relativistic partition function of a system of electrons moving in a fixed potential $V(\mathbf{r})$ is then an integral over their positions:

$$Z \propto \int \prod_i (2\pi mkT)^{3/2} d^3\mathbf{r}_i \exp\left(-\frac{\beta e^2}{4\pi\varepsilon_0}\sum_{i>j}\frac{1}{|\mathbf{r}_i-\mathbf{r}_j|} + \beta e \sum_i V(\mathbf{r}_i)\right). \tag{78}$$

The HST replaces the Coulomb interaction by an auxiliary electrostatic field $\phi(\mathbf{r})$, with its usual field energy:[63]

$$Z \propto \int D\phi(\mathbf{r}) \exp\left(-\beta \int \tfrac{1}{2}\varepsilon_0|\nabla\phi|^2 d^3\mathbf{r}\right) z[\phi], \tag{79}$$

$$\text{where } z[\phi] = \prod_i (2\pi mkT)^{3/2} \int d^3\mathbf{r}_i \exp(\beta e[-i\phi(\mathbf{r}_i)+V(\mathbf{r}_i)]). \tag{80}$$

There is no time-dependence here; the functional integration $\mathcal{D}\phi$ refers to the spatial dependence of ϕ. We can interpret $z[\phi]$ as the partition function of the electrons in an electrostatic field, and the partition function in Eq. (81) as that of electrons and a field. The relations in Section 2.4 then relate correlation functions of the charge density and

$i\varepsilon_0\nabla^2\phi$, as expected from Poisson's equation. The repulsive nature of the Coulomb interaction leads to a **v**-type field with a factor i in the exponent and a rapidly oscillating integrand — a phase problem. In a bounded system it is possible to make the interaction attractive by adding a diagonal interaction of sufficient size that all Fourier components are negative and the fields are real. However, the shift is proportional to the square of the linear dimensions of the system and enhances short-wavelength fluctuations in the field.[64] The relativistic case has recently been tackled, based on the Dirac equation: the factor i results from a Wick rotation to imaginary time, and a suitable choice of gauge eliminates the scalar potential $i\phi$ in favor of a real vector potential coupled to the current.[65]

3.2. *Heisenberg Model*

The auxiliary field method has been applied to the Heisenberg model (82), to obtain the partition function as

$$ Z \propto \int \prod_i D^3 \mathbf{u}_i(\tau) \exp\left(-\frac{1}{4}\int_0^\beta \sum_{ij} J_{ij}^{-1}\, \mathbf{u}_i(\tau)\cdot\mathbf{u}\,(\tau)\,d\tau\right) \prod_i z[\mathbf{u}_i] \qquad (83) $$

where
$$ z[\mathbf{u}] = \mathrm{Tr}\, \mathsf{T}\, \exp\left(\int_0^\beta (\mathbf{B}+\mathbf{u}(\tau))\cdot\mathbf{S}_\tau\, d\tau\right) \qquad (84) $$

is the partition function of a single spin in a time-dependent magnetic field.[66,67,68] This of course assumes that J_{ij} is positive definite, which can be arranged by the addition of a diagonal term to the Hamiltonian:

$$ H = -\mathbf{B}\cdot\sum_i \mathbf{S}_i - \sum_{ij} \tilde{J}_{ij}\mathbf{S}_i\cdot\mathbf{S} \;+\; N_{\mathrm{spins}}J_0 s(s+1) \;\; \text{with}\;\; \tilde{J}_{ij} = J_{ij} + J_0\delta_{ij}, \qquad (85) $$

where J_0 exceeds the largest eigenvalue of $-J_{ij}$. (This causes fewer difficulties than the equivalent correction in the Coulomb system: if the exchange interactions are of finite range, J_0 is finite in the thermodynamic limit.) Since the field breaks time-reversal symmetry, $z[\mathbf{u}]$ is complex, and useful qMC calculations of the Heisenberg model do not use auxiliary fields. The relations in Section 2.4 then relate correlation functions of $\mathbf{u}_i$ to those of $2\sum_j J_{ij}\mathbf{S}_j$, which has a simple interpretation as the fluctuating molecular field acting on the spin $\mathbf{S}_i$ from its neighbors.

3.3. *One-band Hubbard Model: Choice of Auxiliary Fields*

There is said to be considerable ambiguity in the choice of auxiliary fields for the Hubbard model, with one-, two-, three- and four-field methods in use. We shall call these 1F, 2F, 3F and 4F respectively. (The additional freedom to apply linear transformations, for example using $J^{-1}\mathbf{u}$ as the auxiliary field, is not of great concern here.) Let us start with the standard one-band repulsive Hubbard model (4). The ambiguity arises from two observations. The first is the identity $n_{is}^2 = n_{is}$, which allows description of the interaction in terms of an arbitrary combination of spin and charge fluctuations. The

second is the spin isotropy of $n_{i\uparrow}n_{i\downarrow}$ (which simply counts double occupancy), which allows use of scalar or vector auxiliary fields. This leads to a large family of decompositions, which may even be spatially inhomogeneous. Such exact identities cannot affect the results *if no approximations are made*. However, different formulations will give different results once approximations are made; the choice of formulation may also affect the convergence of a qMC calculation.

Let us first write the interaction term as

$$Un_{i\uparrow}n_{i\downarrow} = \tfrac{1}{4}Un_i^2 - US_{iz}^2 \tag{86}$$

where

$$n_i = n_{i\uparrow} + n_{i\downarrow} \quad \text{and} \quad S_{iz} = \tfrac{1}{2}\left(n_{i\uparrow} - n_{i\downarrow}\right) . \tag{87}$$

The HST then gives the 2F auxiliary Hamiltonian[69]

$$\hat{h}_{uv}(\tau) = -\sum_{ijs} t_{ij}c_{is}^{\dagger}c_{js} - \sum_{i}\left(v_i(\tau)n_i + u_i(\tau)S_{iz}\right) \tag{88}$$

with Gaussian weight

$$\exp\left(-\beta V_0[u,v]\right) = \exp\left(-\int_0^{\beta}\sum_i \left(\frac{1}{4U}u_i^2(\tau) + \frac{1}{U}v_i^2(\tau)\right) d\tau\right). \tag{89}$$

The spin-spin attraction and charge-charge repulsion result in a real field u coupled to the z component of spin and an imaginary field iv coupled to the density.

We can avoid the imaginary term (and resulting phase problem) by using the identity $n_{is}^2 = n_{is}$ to rewrite the interaction as

$$Un_{i\uparrow}n_{i\downarrow} = \tfrac{1}{2}Un_i - 2US_{iz}^2 \tag{90}$$

Applying the HST to this decomposition gives the 1F auxiliary Hamiltonian[43]

$$\hat{h}_u(\tau) = -\sum_{ijs} t_{ij}c_{is}^{\dagger}c_{js} - \sum_i u_i(\tau)S_{iz} \tag{91}$$

where the single auxiliary field, acting as a magnetic field in the z direction, has Gaussian weight

$$\exp\left(-\beta V_0[u]\right) = \exp\left(-\int_0^{\beta}\sum_i \frac{1}{8U}u_i^2(\tau) d\tau\right). \tag{92}$$

This has introduced spurious interaction between equal spins on one site. Functional integration of course repairs the damage; Keiter has shown explicitly how the diagrams corresponding to self-interaction in the Anderson model cancel to each order.[70] A systematic study[71] of all possible Gaussian decompositions in the Hubbard model shows that, to each order in the expansion for the grand potential, self-interaction gives rise to spurious diagrams that are only canceled by higher-order diagrams. Any truncation of

the series to a finite order will then introduce unphysical interactions, as will the SA. For example, the saddle-point solution is the Hartree-Fock state $u_i=U\langle 2S_{iz}\rangle$ only in 2F. The SA in the 2F method gives the correct partition function and leading corrections in the Anderson model in both the atomic and band limits.[72] Here Hamann[38,69] found the important paths for the large U to be those that remain close to the Hartree-Fock minima $\langle S_z\rangle=\pm\frac{1}{2}$ most of the time, with hops between the two minima. The effective action is that of an instanton gas with long-range interactions. (Although the two-field method was used, fluctuations of the v field were ignored on the grounds that they are much faster than spin fluctuations. This can give an incorrect temperature dependence.[73]) A study of a number of different schemes for the Anderson model fails to find one correct in all limits.[74]

The above discussion suggests that the 2F method is to be preferred for analytical work. However, MC calculations will suffer from a phase problem as the auxiliary Hamiltonian is complex. This suggests that the 1F method would be more convenient for numerical purposes. Hirsch has taken this further, noting that the operator $n_{i\uparrow}n_{i\downarrow}$ only has eigenvalues 0 and 1 and hence using a non-Gaussian transformation to introduce Ising auxiliary fields $u_i=\pm a$:[75]

$$\exp(-\Delta\tau U n_{i\uparrow}n_{i\downarrow}) = \frac{1}{2}\sum_{u_i=\pm a}\exp\left[u_iS_{iz} - \frac{1}{2}\Delta\tau U n_i\right]$$

(93)

where
$$a = 2\cosh^{-1}\left[\exp(\Delta\tau U/2)\right].$$

(94)

The discrete sample space is computationally more efficient,[76] and is widely used in qMC simulations of the Hubbard model. Again there is a degree of freedom, allowing a family of discrete transformations with different weighting and magnitude of the two auxiliary field values.[77,78]

The above decompositions appear to introduce uniaxial spin anisotropy, and one of the tasks of functional integration is to restore the symmetry. Approximations such as the SA will break the symmetry,[79] introducing a gap to spin waves in a Hubbard ferromagnet. However, even without making such approximations, we come across a puzzling feature of the above HSTs. Let us consider the one-band Hubbard model on a three-dimensional lattice and assume for the moment that it has a second-order magnetic phase transition at finite temperature, an assertion as yet unproved. As a thought computation, let us investigate the critical exponents. (Hirsch has shown evidence of a finite-temperature antiferromagnetic transition at half filling, but resorted to mean field theory to find T_N.[80]) Spin isotropy implies that the critical behavior will correspond to the $d=3$ Heisenberg ($O(3)$) universality class. On the other hand, the HST has transformed the system into one with a one-dimensional order parameter. The resulting action is a very complicated many-body functional, but the width is finite in the time direction and interactions will be damped at large spatial separations. This would suggest Ising critical behavior. Possible resolutions are that the Ising effective action may be singular or have long-range interactions, or that there is no second-order magnetic

transition at finite-temperature. Indeed, coupling between spin and charge fluctuations may drive the transition first order.[81]

These arguments suggest we use the identity $S_{iz}^2 = \mathbf{S}_i^2/3$, valid for a one-band model, to write the interaction in the manifestly isotropic forms

$$Un_{i\uparrow}n_{i\downarrow} = \tfrac{1}{2}Un_i - \tfrac{2}{3}U\mathbf{S}_i^2 = \tfrac{1}{4}Un_i^2 - \tfrac{1}{3}U\mathbf{S}_i^2 \tag{95}$$

where
$$\mathbf{S}_i = \tfrac{1}{2}\sum_{st} c_{is}^\dagger \, \boldsymbol{\sigma}_{st} \, c_{it} \quad , \tag{96}$$

leading to the 3F and 4F transformations respectively.[82,83] The latter has a real *vector* auxiliary field coupling to the total spin and an imaginary scalar field coupled to the density:

$$\hat{h}_{\mathbf{u}v}(\tau) = -\sum_{ijs} t_{ij}c_{is}^\dagger c_{js} \sum_i \left(iv_i(\tau)n_i + \mathbf{u}_i(\tau)\cdot\mathbf{S}_i \right). \tag{97}$$

The effective action is now explicitly isotropic and remains so even after approximations such as the SA, or more generally after discretization in the time direction. On the other hand, the SA no longer gives the Hartree-Fock ground state. In a qMC simulation, a phase problem arises from the spins, as will be shown. The 3F and 4F methods have therefore rarely been used in qMC work, although results on small systems agree with exact diagonalization.[84]

The difference between scalar and vector fields is well illustrated by an intermediate method.[46] The argument is that transverse spin fluctuations are slow (with characteristic frequencies given by the spin wave spectrum), while longitudinal fluctuations are fast (with characteristic frequencies of the order of the band width). The interaction is therefore referred to a local spin quantization direction:

$$Un_{i\uparrow}n_{i\downarrow} = \tfrac{1}{2}Un_i - 2U(\mathbf{e}_i\cdot\mathbf{S})^2 = \tfrac{1}{4}Un_i^2 - U(\mathbf{e}_i\cdot\mathbf{S})^2 \tag{98}$$

where $\mathbf{e}_i$ is a time-independent (but site-dependent) unit vector. The auxiliary field $u_i\,\mathbf{e}_i$ is of fixed direction (but fluctuating magnitude) on each site. The partition function $Z(\{\mathbf{e}_i\})$ is calculated and averaged over the directions. Clearly the exact partition function is independent of our local choice of quantization axis, and the averaging is unnecessary in an exact calculation. In the SA the partition function *does* depend on the (unsigned) directions. This is seen most clearly by consideration of the ground state energy $E_{\text{SA}}(\{\mathbf{e}_i\})$. Suppose the Hartree-Fock ground state is a ferromagnet or a collinear antiferromagnet. The ground state found by the 2F SA is only the Hartree-Fock state when all the $\mathbf{e}_i$ are collinear. A further ambiguity arises in the Jacobian in the integral for the SA; in 3F the volume element is $d^3\mathbf{u}_i$, while in 1F the volume element is $d\mathbf{e}_i du_i$.[85] A similar idea, involving integration over local constraints in direction, has also been used in the first-principles spin density functional theory of the statistical mechanics of iron.[86]

We have so far implicitly assumed that we are looking for magnetism. The upsurge of interest in the Hubbard model in recent years has been due to its possible relevance to cuprate superconductivity. This suggests yet another decomposition into pairing opera-

tors, coupled to a particle non-conserving auxiliary field.[87,88,89] A general decomposition involving both spin and pairing operators has been proposed.[90]

Fermion determinants and Green functions are calculated as in Section 2.4. For example, the auxiliary Hamiltonian in the 4F method has matrix elements

$$h_{isjt}(\tau) = -\left(t_{ij}\delta_{st} + iv_i(\tau)\delta_{st}\delta_{ij} + \tfrac{1}{2}\mathbf{u}_i(\tau)\cdot\boldsymbol{\sigma}_{st}\delta_{ij} + \mu\delta_{ij}\delta_{st} \right) . \tag{99}$$

Now if all the $\mathbf{u}_i(\tau)$ are collinear, as in 2F, the matrix is block-diagonal in spin "up" and "down" blocks, and the determinant decouples into a product of spin "up" and "down" determinants. In general, with non-collinear fields, this is not possible.

For later use, we generalize the distinction between scalar and vector auxiliary fields. To make the definitions more precise, consider the operators $\hat{A}_\mu$ coupled to the auxiliary field. If these operators commute at equal time, such as S_{iz} and n_i in 2F, we talk of a *scalar* field. If the operators do not commute, as in 3F and 4F and the spin components in the Heisenberg model, we talk of a *vector* field.

3.4. *Many-band Hubbard model*

Our freedom choice of auxiliary-field representation is much reduced in N-band Hubbard models if we require the number of auxiliary fields to be independent of N. This reduces the freedom of choice provided by the identities in the single-band model. Let us first consider the attractive (negative U) $SU(N)$ Hubbard model (5), known to have no sign problem. In this case we only require a one-component field u_i coupling to the density on each site; the auxiliary Hamiltonian is then

$$\hat{h}_u^{(N)}(\tau) = \sum_{a=1}^{N} \left(-\sum_{ij} t_{ij} c_{ia}^\dagger c_{ja} - \sum_i u_i(\tau)\left(n_{ia} - \tfrac{1}{2}\right) \right) \tag{100}$$

with Gaussian weight

$$\exp\left(-N\beta V_0[u]\right) = \exp\left(N\int_0^\beta \sum_i \frac{1}{4U} u_i^2(\tau)\, d\tau \right). \tag{101}$$

The auxiliary partition function of the electrons is simply related to that for $N=1$:

$$z^{(N)}[u] = \mathrm{Tr}\, \mathsf{T}\exp\left(-\int_0^\beta h^{(N)}(\tau)\, d\tau\right) = \left(z^{(1)}[u]\right)^N . \tag{102}$$

The partition function is then

$$Z = \frac{\int \prod_i \mathsf{D}u_i(\tau)\ \exp\left(-N\beta V[u]\right)}{\int \prod_i \mathsf{D}u_i(\tau)\ \exp\left(-N\beta V_0[u]\right)} \tag{103}$$

where $\qquad\qquad\qquad V[u] = V_0[u] - kT\, \ln z^{(1)}[u] . \tag{104}$

The free energy must be independent of U when $N=1$, apart from a constant $U/4$ per atom, since there is no interaction. This is not obvious from the functional integral form.

Now the auxiliary field is time-reversal invariant, so that $z^{(1)}[u]$ must be real (but not necessarily positive). There is therefore no sign problem for N even. We shall see an explicit construction of a sign problem for N odd in Section 6. The situation is different in the $SU(N) \infty SU(2)$ Hamiltonian (105). Since the auxiliary field couples to spin, time-reversal invariance is broken and there is in general a phase problem.

4. The phase problem

In the general situation the auxiliary fields break time-reversal invariance and the weight w of a path is therefore complex. If the quantity to be averaged is real, the real part of the weight suffices. If the phase of a typical path is much less than $\pi/2$, as may be the case at high temperatures, the average sign will be close to unity and the phase problem will not seriously affect numerical convergence. Phase fluctuations will increase with increasing imaginary time.[91]

The phase of a path in the functional integral has a geometrical interpretation. We therefore review the theory of the geometrical (Berry) phase, [92,93] before applying it to the functional integral.

4.1. *Geometrical phases*

Suppose a Hamiltonian H depends on parameters $\mathbf{R}$ in some parameter space $\mathcal{F}$, and has eigenstates $\{|n; \mathbf{R}\rangle\}$ for each point $\mathbf{R}$:

$$H(\mathbf{R}) \, |n; \mathbf{R}\rangle = E_n(\mathbf{R}) \, |n; \mathbf{R}\rangle \, . \tag{106}$$

(One example is the Born-Oppenheimer approximation for a molecule, where $\mathbf{R}$ are nuclear coordinates and H is the electron Hamiltonian; another example is a spin s particle in a magnetic field $\mathbf{R}$.) Prepare the system in the nth eigenstate $|\Psi(0)\rangle = |n; \mathbf{R}(0)\rangle$ at time 0 and take $\mathbf{R}$ slowly round a closed path C in $\mathcal{F}$ in (real) time T. If the state remains non-degenerate, it will evolve nearly adiabatically. The final state will be the same as the initial state, the final wave function differing by a phase factor from the initial wave function:

$$|\Psi(T)\rangle = \exp\left(-\frac{i}{\hbar}\int_0^T E_n(\mathbf{R}(t)) \, dt\right) \exp(i\gamma_n(C)) \, |\Psi(0)\rangle \, . \tag{107}$$

The first exponent is simply the dynamical phase expected from the time-dependent frequency of the system. The second exponent (whose general nature escaped attention before the 1980s) is the *Berry phase*

$$\gamma_n(C) = \oint \mathbf{A}_n(\mathbf{R}) \cdot d\mathbf{R} \, , \text{ where } \mathbf{A}_n(\mathbf{R}) = i \, \langle n; \mathbf{R} | \nabla_{\mathbf{R}} | n; \mathbf{R} \rangle \, , \tag{108}$$

a geometrical property of the path in parameter space. If the $\mathbf{R}$ variables are quantized, $\mathbf{A}_n(\mathbf{R})$ becomes a gauge potential; if the system separates into fast and slow variables

(such as electronic and nuclear degrees of freedom), this potential appears in the Hamiltonian of the slow variables after elimination of the fast variables.

Aharonov and Anandan generalized Berry's argument to non-adiabatic evolution by viewing the dynamics in state space rather than parameter space.[94] The wave function is a vector $|\Psi\rangle$ in *Hilbert space* $\mathcal{H}$. All wave functions in the ray $c|\Psi\rangle \in \mathcal{H}$, where $|\Psi\rangle$ is a fixed normalized wave function and c is a non-zero complex number, correspond to the same state in *state space* $\mathcal{P}$. Points in $\mathcal{P}$ are therefore equivalence classes of wave functions, or normalized projection operators $|\Psi\rangle\langle\Psi|$. The geometrical phase depends only on the path in state space and the curvature of that space. It does not depend on the Hamiltonian, or on the adiabaticity of the evolution, or — important for our present purposes — on whether the path is parametrized by real or imaginary time. It is often described in the language of fiber bundles:[95] the fiber above any state in $\mathcal{P}$ contains the allowed wave functions $c|\Psi\rangle$. A closed path in state space need not return to a wave function of the same point in the fiber.

4.2. *Heisenberg model*

The phase problem in qMC is closely related to these geometric phases.[96] Let us consider the Heisenberg model as discussed in section 3.2, where the weight of a path involves the partition function of $z[\mathbf{u}]$ of independent spins in an imaginary-time-dependent magnetic field $\mathbf{u}_i(\tau)$. This partition function is the trace of the time-evolution operator

$$\hat{U}(\tau) = \mathsf{T}\prod_i \, \exp\!\left(\int_0^\beta \mathbf{u}_i(\tau)\cdot\hat{\mathbf{S}}_{i\tau}\, d\tau\right),$$

(109)

which is not unitary, but (in this case) has determinant 1. It is the solution of the differential equation

$$\frac{d}{d\tau}\hat{U}(\tau) = \sum_i \mathbf{u}_i(\tau)\cdot\hat{\mathbf{S}}_{i\tau}\,\hat{U}(\tau) \ \ \text{with} \ \ \hat{U}(0) = 1.$$

(110)

As it decouples into a product of single-site operators, we only need consider the effect on a single spin. However, the differential equation cannot be integrated in closed form for an arbitrary time dependence even for a single spin $\frac{1}{2}$. It can be visualized as dynamics of coherent states as unit vectors $\mathbf{n}$ on the Bloch sphere, as described in Section 2.2.[97] While the *real-time* dynamics of a spin in a real magnetic field is precession around a field, the *imaginary-time* dynamics is relaxation towards the field. In the language of Section 4.1, Hilbert space $\mathcal{H}$ is $\mathbb{C}^2$, the space of two-component spinors, and state space $\mathcal{P}$ is the (Bloch) sphere S^2. The auxiliary field $\mathbf{u}$ moves in a parameter space (or field space) $\mathcal{F} = \mathbb{R}^3$.

First consider a spin $\frac{1}{2}$ in a *static* field $\mathbf{u}\neq\mathbf{0}$. The ground state in the field is $\hat{\mathbf{u}}$, the unit vector parallel to $\mathbf{u}$. We use $|\mathbf{u}\circledR$ to denote the corresponding normalized ground state wave function, defined up to a phase for all non-zero $\mathbf{u}$. The time evolution operator is then

$$\hat{U}(\tau) = e^{u\tau/2}|\hat{\mathbf{u}}\rangle\langle\hat{\mathbf{u}}| + e^{-u\tau/2}|-\hat{\mathbf{u}}\rangle\langle-\hat{\mathbf{u}}|\,, \tag{111}$$

which becomes an unnormalized projection onto the ground state as $\tau \oslash \infty$. If the initial angle between the state $\mathbf{n}$ and the field $\mathbf{u}$ is $\alpha(0)$, so that $|\langle\mathbf{u}|\mathbf{n}\rangle| = \cos\frac{1}{2}\alpha(0)$, time evolution is relaxation along the great circle containing $\mathbf{n}$ and $\hat{\mathbf{u}}$, with

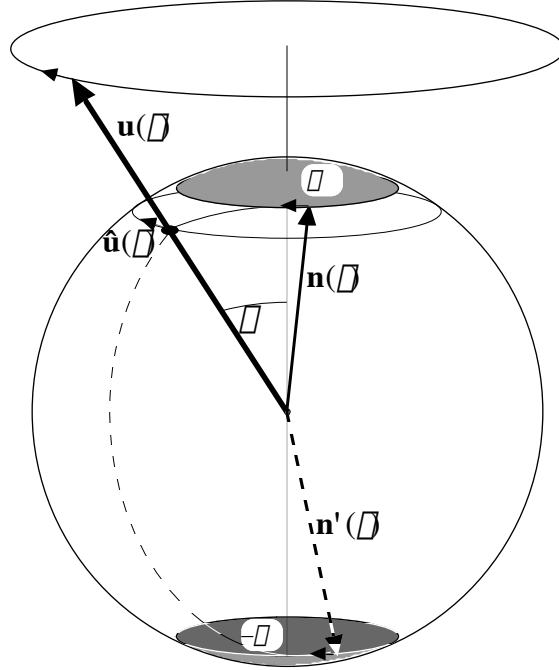$$\tan\tfrac{1}{2}\alpha(\tau) = \tan\tfrac{1}{2}\alpha(0)\,e^{-u\tau}. \tag{112}$$

Fig. 2. The dynamics of a spin in an imaginary-time-dependent field $\mathbf{u}(\tau)$. Full lines represent the eigenvector $\mathbf{n}$, its path on the sphere and the great circle along which it relaxes; dashed lines represent these for $\mathbf{n}'$.

With a time-dependent field this becomes a pursuit problem on the sphere. The spin direction moves along a great circle towards the instantaneous ground state. In general the dynamics of the auxiliary field is discontinuous, and that of the state is non-differentiable but continuous. The state evolution therefore describes a curve on the sphere. Diagonalization of the evolution operator $\hat{U}(\beta)$ yields two time-dependent eigenstates $\mathbf{n}(\tau)$ and $\mathbf{n}'(\tau)$ that describe closed paths on the sphere, enclosing solid angles Ω and $-\Omega$ respectively, as illustrated for a conical path in Fig. 2. The wave functions acquires geometrical phase factors $\pm\frac{1}{2}\Omega$ that depends only on the solid angle $\pm\Omega$ enclosed by this closed path, and not on the dynamics on the path or even whether it is parametrized by real or imaginary time. The partition function of this path is[96]

$$z[\mathbf{u}] = R[\mathbf{u}]e^{i\Omega/2} + R[\mathbf{u}]^{-1}e^{-i\Omega/2} \tag{113}$$

where the real amplitude factor

$$R[\mathbf{u}] = \exp\left(\int_0^\beta \tfrac{1}{2}\mathbf{u}(\tau)\cdot\mathbf{n}(\tau)d\tau\right) \tag{114}$$

does depend on the dynamics. At high temperatures there is insufficient time for the spin to evolve far; it responds to the time-averaged field, recovering the SA. At low temperatures, the state can follow a smooth field path almost adiabatically; the phase is then a Berry phase. There is thus a mapping between field paths in the auxiliary-field integral and spin paths in the coherent-state integral of section 2.2. The phase problem in the auxiliary-field method is simply the Berry phase S_{WZ} discussed there.

When the functional integral is discretized, the phase problem increases in severity with the number L of time slices. In the static approximation there is a single time slice, and the spin paths are the points $\pm\hat{\mathbf{u}}$, which do not enclose area and therefore have zero phase. With $L=2$, the spin paths are great circle arcs in the plane containing the two auxiliary field values, and the enclosed area and phase vanish similarly. In algebraic terms, this is the result that Tr $\exp(-\beta\mathbf{u}\cdot\mathbf{S})$ and Tr $\{\exp(-\tfrac{1}{2}\beta\mathbf{u}_2\cdot\mathbf{S})\exp(-\tfrac{1}{2}\beta\mathbf{u}_1\cdot\mathbf{S})\}$ are real. With $L=3$ (or greater), the spin describes a spherical triangle (or polygon) which can enclose area and have non-zero phase.[98] In the continuum limit, the effective action $-\ln w$ is highly non-local in time, but can be expanded in the auxiliary field.[99] The phase manifests itself as a magnetic monopole potential for this field.

4.3. *Generalization*

Let us now turn to the Hubbard model. The 1F and discrete transformations described in Section 3.3 can give a real auxiliary Hamiltonian, and therefore a real (but not necessarily positive) weight. The 3F and 4F methods, used to maintain symmetry, result in a complex weight. The physical picture is that a large auxiliary field making a closed path on one site would transport the local magnetization in such a way as to give a geometrical phase. With more realistic on-site interactions in a many-electron atom, such as in the $SU(N)\times SU(2)$ Hubbard model (115), we no longer have the freedom to use a scalar field; conversely, the interaction term $\sum_a n_{ia\uparrow}n_{ia\neg}$ breaks spin isotropy for $N>1$. We are forced to use vector fields. There have been qMC studies of three-band Hubbard models of cuprate superconductors, describing d orbitals on Cu sites and p orbitals on O sites.[100,101] The simulations include hybridization but neglect inter-band exchange interactions, and can therefore resort to scalar fields. As more realistic systems are tackled in the future, the phase problem is likely to become increasingly relevant.

Consideration of a general model with local interactions between degenerate orbitals illustrates the need for vector fields. In the atomic limit there is an interaction, as in Eq. (116), but no hopping term. If a scalar field HST is possible, all terms in the auxiliary Hamiltonian commute and the functional integral can be replaced by an ordinary integral. The ground state is then a single Slater determinant, the Hartree-Fock state. This is the correct answer for the one band Hubbard model in the atomic limit, but in general the

true ground state is not the Hartree-Fock approximation. A vector field is therefore required if one is to recover the correct atomic physics.

Systems such as these may suffer from more intractable phase or sign problems than those with scalar fields for a variety of reasons. Firstly, the phase for a spin has physical content as discussed in Section 2.2: it encodes spin quantization and the subtleties of low-dimensional antiferromagnets, and should therefore appear in a simulation.

Secondly, we can consider the distribution of the auxiliary field. Since all cumulants of operators and fields apart from the second cumulant (117) are equal up to a linear transformation, we can encode these relations as a relation between the probability distribution for the operators and that for the auxiliary fields.[102] The field distribution is a Gaussian convolution of the operator distribution; the latter in turn is related to the *Wigner function*, a joint distribution for non-commuting variables that cannot be positive definite.[103] Let us integrate all finite-frequency Fourier components out of the functional integral. This gives a classical effective Hamiltonian $V_{\text{eff}}(kT \int \mathbf{u} d\tau)$ for the time-averaged field, containing quantum corrections to V_{SA} to all orders.[14] Under certain circumstances (a field coupled to a conserved order parameter at low temperature) the averaged auxiliary field weight $\exp(-\beta V_{\text{eff}})$ becomes a Wigner function. This result, that even after averaging out all non-zero frequency fluctuations, the weight can still be negative, suggests a serious sign problem for vector fields. The physical interpretation here is that the qMC simulation is attempting to find simultaneous values for incompatible variables, for example all components of a spin. The sign problem is a consequence of the impossibility of this quest. It occurs if the operators coupled to the auxiliary field generate a non-Abelian symmetry group; that is, they commute with the Hamiltonian but not with each other. This is necessary if the simulation is to study the total magnetization of an isotropic model, such as the Heisenberg or Hubbard model.

Finally, let us consider the commutator of the operators appearing in the auxiliary Hamiltonian:

$$\left[\hat{A}_\mu(\tau), \ \hat{A}_\nu(\tau') \right] \sim (\tau - \tau')^n. \tag{118}$$

In this commutator the explicit time dependence of the operators is taken with respect to the auxiliary Hamiltonian $h_{\mathbf{uv}}(\tau)$. With a vector field, the equal-time commutator is non-vanishing, giving $n=0$. With a scalar field, n will be greater than zero and the weight might be expected to be more "classical".

How does the geometrical picture apply to more general Hamiltonians? It has also been noted in fermion systems.[104] Let us suppose initially that there is only a **u** field. The time evolution operator $\hat{U}_{\mathbf{u}}(\tau)$ acts on wave functions in Hilbert space $\mathcal{H}$. Each (static) value of the auxiliary field then has a ground state submanifold $p(\mathbf{u}) \wp \mathcal{P}$ (a point if the ground state is non-degenerate). Then in the $\tau \oslash \infty$ limit, the evolution projects the state onto p. (If there is a **v** field, the dynamics is partly relaxational and partly unitary.) In a time-dependent field, the state will relax towards the instantaneous p and move along a path in $\mathcal{P}$. If $\hat{U}_{\mathbf{u}}(\beta)$ is now diagonalized, its eigenstates will describe closed paths with well-defined geometrical phases. (Strictly, as $\hat{U}$ is not a normal matrix, it need not have a

complete set of eigenstates if there are degenerate eigenvalues.[105] We shall assume that the eigenstates do form a complete set for almost all paths.)

5. The sign problem

When the auxiliary Hamiltonian $h_{uv}(\tau)$ is real, the weight of all paths must be real. One example is the XY model, where the auxiliary field couples to two spin components (S_x and S_z if one wishes to keep everything real). Others include the 1F and discrete transformations in the Hubbard model. However, this only guarantees that the weight is real; it may oscillate rapidly in sign. There remains the question of whether the average sign of the paths remains bounded away from zero in the low-temperature limit.

5.1. *Origin of the sign problem*

The sign problem has been more widely discussed in the literature than the phase problem, as complex Hamiltonians are usually avoided if possible in qMC calculations. Blankenbecler *et al*, in their studies of coupled fermion-boson systems, appear to have been the first to remark on both.[53] They argued that rapidly fluctuating boson fields were responsible for the problem. These fluctuations are suppressed by time derivatives in the boson action in their model. However, no such time derivative appears in the action for auxiliary fields and the fluctuations are correspondingly larger.

The sign problem can arise from Fermi statistics. Loh *et al* considered the evolution of the many-electron wave function in the time-dependent auxiliary field.[106] Their picture is of electron world lines encircling each other. If the total winding number is odd, the weight $w[\mathbf{u}, \mathbf{v}]$ of the path is negative. They argue that the number of exchanges is proportional to the imaginary time, so that the average sign

$$s_{av} = \frac{\int \mathsf{D}^{n_+}\mathbf{u}(\tau)\, \mathsf{D}^{n_-}\mathbf{v}(\tau)\, w[\mathbf{u},\mathbf{v}]}{\int \mathsf{D}^{n_+}\mathbf{u}(\tau)\, \mathsf{D}^{n_-}\mathbf{v}(\tau)\, |w[\mathbf{u},\mathbf{v}]|}$$

(119)

should tend to zero exponentially as $e^{-\beta\Delta}$, where Δ is a constant. This is indeed what they find in simulations of the Hubbard model away from half filling. Sorella has proved that s_{av} either remains bounded away from zero or falls exponentially to zero in the low-temperature limit.[61] He proposes ignoring the sign, taking averages with respect to $|w|$, and shows that the ground state energy calculated in this way is $E_0 - \Delta$. Measurement of the temperature dependence of the sign therefore allows correction of the ground state energy. Unfortunately, other quantities such as the pair susceptibility are incorrect at low temperatures if the sign is neglected.[106] The Hamiltonian that is being simulated is different from the true Hamiltonian, and may have lost some physical content. The same situation occurs in a very different context: path integral simulations of homonuclear diatomic molecules on a surface.[107] Here the sign reflects the Fermi or Bose statistics of the atoms, and has a large effect for light molecules.

Some authors have discussed the sign problem in the Hubbard model, in particular in projector qMC, in terms of wave function dynamics in Hilbert space. With a real HST such as the discrete transformation in Eq. (120) the wave functions remain real and we can restrict consideration to a real Hilbert space. As a single auxiliary field cannot introduce correlations, the space of Slater determinants is invariant under time evolution in an auxiliary field. In the projector method, the starting state Ψ_T may be the Hartree Fock ground state, which will evolve in this space under the influence of an auxiliary field. Functional averaging of the Slater determinants then yields the correlated many-electron state. Fahy and Hamann interpret this as a diffusion process (with drift and decay terms), deriving a transport equation for the distribution $f(\Psi; \tau)$ of wave functions.[108] Since this equation is symmetric under inversion $\Psi \varnothing - \Psi$, eigenfunctions of the diffusion operator have even or odd parity. The slowest decaying eigenfunction has even parity, giving equal weight to Ψ and $-\Psi$, corresponding to a vanishing many-body wave function. The first odd-parity eigenfunction, the solution of physical interest, decays more rapidly. The difference between the decay rates gives the decay rate Δ. The authors have developed a positive projection method, requiring that Ψ not cross a nodal surface on which it is orthogonal to a trial function. This allows a better approximation to the odd parity solution, and hence the correct ground state.[109]

Muramatsu *et al* interpret the sign problem in terms of topological properties of the manifold of Slater determinants.[110] The one-electron basis functions making up a Slater determinant define a set of orthogonal axes (a point in a Stiefel manifold). The physical state depends only on the hyperplane spanned by these axes (a point in a Grassmannian manifold). The hyperplane at the $\tau = \beta$ is projected onto the initial hyperplane. The rotation required to restore the axes to their original orientation is either proper or improper. In the latter case, the path has negative weight.

There have been further proposals for the class of path responsible for the sign problem. One recent suggestion is that topological solitons in the auxiliary field, antiferromagnetic domain walls propagating in imaginary time, have negative weight, although this is unlikely to be a major source of the problem.[111]

5.2. *Absence of a sign problem*

There are a few systems in which the sign problem is absent, usually as a consequence of symmetry. One well-known example with positive weight is the *negative-U* Hubbard model, as already discussed in Section 3.4: the weight $(z^{(1)}[\mathbf{u}])^N$ is positive for even N. In the half-filled *positive-U* Hubbard model on a bipartite lattice, with a discrete HST, the weight is also non-negative: the fermion determinant separates into the product of spin-up and spin-down determinants, which have the same sign due to particle-hole symmetry.[112] The weight can still vanish where the fermion determinant vanishes, and care is needed to ensure the simulation is ergodic and is not trapped inside a nodal surface.[113] The negative signs reappear away from half filling, but are not monotonic functions of the doping.[54,62]

Batrouni and de Forcrand have proposed a discrete HST that does yield a positive fermion determinant z in the Hubbard model for arbitrary filling.[77] However, this re-

quires the weight of one of the two discrete values of the auxiliary field to become negative. While this does not solve the sign problem, it is at least known which field configurations have negative weight. In conventional simulations, this only emerges once the determinant has been computed.

Sorella has proposed symmetrizing the HST;[114] instead of integrating over a single sample of paths, one averages the contribution from $+u_{\mu l}$ and $-u_{\mu l}$ in each time slice. This is equivalent to replacing $\exp(u_{\mu l}\hat{A}_\mu\Delta\tau)$ in Eq. (121) by $\cosh(u_{\mu l}\hat{A}_\mu\Delta\tau)$. The sign problem is then absent in the limit of many time slices L; however, as the number of paths sampled grows as 2^L, this has not yet been shown to be a practical solution.

It has recently been shown that the sign problem is absent in the grand canonical ensemble for certain types of Hamiltonian, in which the one-body term is time-reversal invariant and the only interactions are attractive interactions between an operator and the its time-reversed counterpart.[115] The eigenvalues of the evolution matrix then appear in complex conjugate pairs. Their time-reversal operation T (translated from their original application to the nuclear shell model) has the effect

$$\left.\begin{array}{ll} T\,c_{i\uparrow}^\dagger = -c_{i\downarrow}^\dagger; & T\,c_{i\downarrow}^\dagger = c_{i\uparrow}^\dagger \\ T\,c_{i\uparrow} = -c_{i\downarrow}; & T\,c_{i\downarrow} = c_{i\uparrow} \end{array}\right\} \quad . \tag{122}$$

The usual Hubbard interaction $Un_{i\uparrow}n_{i\neg}$ is therefore time-reversal invariant. An immediate consequence of their theorem is the absence of the sign problem in the negative-U one-band Hubbard model. Their method suggests a solution of the phase problem in the Heisenberg model. The spin operators S_x and S_z change sign under the time reversal operation but S_y does not. It is possible to write the isotropic spin $\frac{1}{2}$ Heisenberg model (with external field in the xz plane) in such a form by adding appropriate self-interactions:

$$-\sum_{ij} J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j = -\sum_{ij}\left[\tilde{J}_{ij}^X\left(S_{ix}S_{jx}+S_{iz}S_{jz}\right)+\tilde{J}_{ij}^Y S_{iy}S_{jy}\right] + N_{\text{spins}}\left(\tfrac{1}{2}J_0^X+\tfrac{1}{4}J_0^Y\right), \tag{123}$$

where
$$\tilde{J}_{ij}^X = J_{ij} + J_0^X\delta_{ij} \text{ and } \tilde{J}_{ij}^Y = J_{ij} + J_0^Y\delta_{ij}. \tag{124}$$

In Eq. (125), $J_0^X{=}J_0^Y$ was positive and chosen sufficiently large that the matrix $\tilde{J}^X{=}\tilde{J}^Y$ became positive-definite. The integrand is then complex: there is a phase problem (Section 4.2). The alternative is to use the same positive value of J_0^X, and a sufficiently large *negative* J_0^Y, so that the matrix $\tilde{J}^Y$ is the negative block of the interaction. The auxiliary Hamiltonian

$$\hat{h}_{\mathbf{uv}}(\tau) = -\sum_i\left[\left(B_x+u_x(\tau)\right)\mathbf{S}_{ix\tau} + iv_y(\tau)\mathbf{S}_{iy\tau} + \left(B_z+u_z(\tau)\right)\mathbf{S}_{iz\tau}\right] \tag{126}$$

is then real, as the imaginary σ_y matrix is multiplied by an imaginary quantity. We have eliminated the phase problem at great cost to the esthetics and symmetry of the Hamilto-

nian. Unfortunately, the theorem only applies to fermions in the grand canonical ensemble and a sign problem still remains.

6. A simple example: a triangular molecule

It is sometimes stated that the sign problem is a consequence of Fermi statistics, or of spin. A trivial example illustrates many of the above features and interpretations of the sign problem for a single spinless particle, albeit with frustration. Consider the attractive $SU(N)$ Hubbard model (127) on a three-site lattice with periodic boundary conditions and *negative* hopping integrals $t_{ij} = -1$ — or equivalently, positive hopping integrals and threaded by half-integer magnetic flux. To find the weight of paths, we only need consider $N=1$. We consider third filling (one particle). The dynamics is clear: each time its world line encircles the loop, the wave function changes sign. We will see how an auxiliary field performs this transport and relate it to the foregoing discussions.

The matrix (h_{ij}) representing the auxiliary Hamiltonian (128) is

$$h = \begin{pmatrix} -u_1 & 1 & 1 \\ 1 & -u_2 & 1 \\ 1 & 1 & -u_3 \end{pmatrix}. \tag{129}$$

We can take $u_1 + u_2 + u_3 = 0$ without loss of generality. In zero field, the ground state is a doublet of right and left traveling waves

$$|+\rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ e^{2\pi i/3} \\ e^{4\pi i/3} \end{pmatrix}, |-\rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ e^{4\pi i/3} \\ e^{2\pi i/3} \end{pmatrix} \tag{130}$$

of energy -1; there is an excited state of energy 2. The auxiliary field lifts this degeneracy. For small fields we can restrict to the ground state doublet and transform to a pseudospin system. Let us define the symmetry-breaking fields

$$\left. \begin{array}{l} B_x = -\frac{1}{2}(u_2 + u_3) \\ B_y = \frac{1}{2\sqrt{3}}(u_3 - u_2) \end{array} \right\}. \tag{131}$$

The auxiliary Hamiltonian in the basis $|+\rangle, |-\rangle$ is

$$h = \begin{pmatrix} -1 & (\frac{1}{2} - \frac{i}{2\sqrt{3}})u_2 + (\frac{1}{2} + \frac{i}{2\sqrt{3}})u_3 \\ (\frac{1}{2} + \frac{i}{2\sqrt{3}})u_2 + (\frac{1}{2} - \frac{i}{2\sqrt{3}})u_3 & -1 \end{pmatrix} = -1 - \mathbf{B} \cdot \boldsymbol{\sigma}. \tag{132}$$

(The z component of the symmetry breaking field, diagonal in the basis, corresponds to an additional flux threading the loop rather than to an auxiliary field.) Now if this field takes a closed path winding once round the degeneracy, and the state follows adiabatically, we have the classic example of a Berry phase.[92] Figure 3 illustrates the dynamics

of the wave function; Berry gives similar examples related to nuclear motion and to deformations of a triangular membrane.[116]
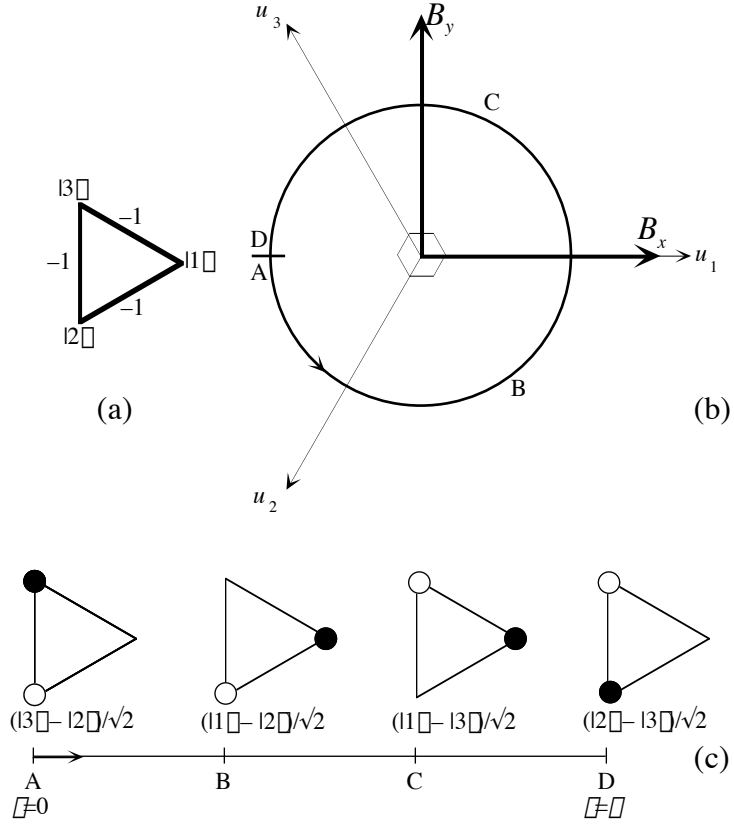

Figure 3. (a) A triangular molecule. (b) A cyclic evolution of the auxiliary field encircling the degeneracy. (b) Evolution of the wave function. Circles represent amplitude: a black circle is positive, a white one negative.

The figure shows a projection of the auxiliary field space $\{u_1, u_2, u_3\}$ onto the plane $u_1+u_2+u_3 = 0$, which is normal to the line of degeneracies $u_1=u_2=u_3$. The axes B_x and B_y, as defined above, are shown; B_z is not in this space. The field is taken once round the circle A∅B∅C∅D=A sufficiently slowly that the particle follows nearly adiabatically. At $\tau=0$ (point A) the auxiliary field is $\mathbf{u} = (-\varepsilon, \ \varepsilon/2, \ \varepsilon/2)$, where $\varepsilon>0$. The ground state wave function, as indicated, is $(|3⑧-|2⑧)/\sqrt{2}$. The solution for adiabatic evolution of this function is

$$|\psi(\tau)\rangle = \sqrt{\frac{2}{3}} \begin{pmatrix} \sin(\pi\tau/\beta) \\ \sin(\pi\tau/\beta-2\pi/3) \\ \sin(\pi\tau/\beta+2\pi/3) \end{pmatrix} e^{(1+\varepsilon/2)\tau} \quad . \tag{133}$$

(The adiabatic assumption is not strictly necessary. The time-dependent eigenstates for large $\beta\varepsilon$ restricted to the two-state system correspond to the above with a phase lag vanishing in the adiabatic limit.) As the field moves to B, where $\mathbf{u} = (\varepsilon/2, \varepsilon/2, -\varepsilon)$, the amplitude shifts from site 3 to site 1, but the amplitude at site 2 remains negative. The crude physical picture is then of a bond being flipped round the edges of a triangle, keeping one end fixed at each flip. After one cycle the orientation of the bond is reversed. The wave function has changed sign, and the auxiliary partition function $z^{(1)}[\mathbf{u}]$ is negative. We can therefore have negative weight in the attractive $SU(N)$ Hubbard model for odd N.

This system has been extensively studied in molecular physics and is the textbook example of an $E \otimes \varepsilon$ Jahn-Teller effect in triangular molecules.[117] The sign change resulting from the adiabatic evolution of a Hamiltonian around a degeneracy in parameter space has long been recognized,[118] and the resulting fractional quantization of the rotational-vibrational spectrum has been observed in Na_3 clusters.[119]

Let us now analyze this instance of the sign problem in terms of the interpretations of Sections 4 and 5. Firstly, it appears directly as a Berry phase due to the evolution of a Hamiltonian around a degeneracy, although recognition of this effect long predates the Berry phase. This is, by explicit construction, the same as the evolution of a spin $\frac{1}{2}$ in an auxiliary field in the equatorial plane illustrated in Fig. 2.

We can also relate this to the topological interpretation described in Section 5.[110] In this case the manifold of normalized Slater determinants is the manifold of unit vectors in three dimensions — the sphere S^2 but not the Bloch sphere — and the state space is the manifold of unoriented rays through the origin, or the sphere with antipodes identified. The path in Figure 3 is a circle in parameter space, but (if the amplitude factor is removed) a semicircle in Hilbert space. At the end of the time evolution, as the ray returns to itself a sign change in the wave function has occurred.

How does this generalize? The example is too simple to have direct application. However, the linear dependence of the ground state energy on the auxiliary field suggests the possibility of symmetry breaking (in a mean field approximation), analogously to the Jahn-Teller effect. The extension to the Hubbard model on triangular lattices or the possible relevance to flux phases remains to be seen. The system is also related to the sign problem occurring in world-line qMC simulations of the Heisenberg antiferromagnet on a triangular lattice.[120] In this case the paths giving negative signs involve a sequence of spin flips encircling a frustrated plaquette.

7. Prospects

This review article has attempted to put the extensive literature on quantum Monte Carlo simulations, auxiliary field functional integration and the occurrence of the sign problem into a general context. As such, the author gives the usual apologies to those whose relevant contributions have inadvertently been overlooked.

Some readers may have started with this paragraph to see how the sign problem has been solved in the auxiliary-field method. They will be disappointed. In Section 5, we

have seen a number of situations in which the sign problem is indeed absent, and a number of proposals for its circumvention in other cases. Sometimes a judicious choice of the auxiliary fields suffices, possibly at the cost of the apparent symmetry. However, it is likely to be a more serious impediment in systems with more complicated local interactions than usually studied, specifically where Hartree-Fock does not give the true ground state the atomic limit. A vector auxiliary field is necessary here and a phase problem appears to be inevitable, a consequence of the attempt of the simulation to violate the uncertainty principle. A proper understanding of the origin of this problem is needed if it is to be alleviated and low temperature calculations performed.

8. References

1. R. L. Stratonovich, *Sov. Phys. Dokl.* **2**, 416 (1957); J. Hubbard, *Phys. Rev. Lett.* **3**, 77 (1959).
2. See, for example, *Electron Correlation and Magnetism in Narrow Band Systems*, ed. T. Moriya (Springer Ser. in Solid-State Science, Berlin, 1981) and references therein.
3. S. Levit, *Phys. Rev.* **C21**, 1594 (1980).
4. J. W. Negele and H. Orland, *Quantum Many Particle Systems* (Addison Wesley, Redwood City, 1988).
5. R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw Hill, New York, 1965).
6. L. S. Schulman, *Techniques and Applications of Path Integration* (Wiley, New York, 1981).
7. K. Binder and D. W. Heerman, *Monte Carlo Simulation in Statistical Physics* (Springer, Berlin, 1988) describe the classical algorithms.
8. N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller and E. Teller, *J. Chem. Phys.* **21**, 1087 (1953).
9. M. Suzuki (ed.) *Quantum Monte Carlo Methods in Equilibrium and Nonequilibrium Systems* (Springer, Berlin, 1987).
10. W. von der Linden, *Phys. Rep.* **220**, 53 (1992) gives a recent review.
11. M. C. Gutzwiller, *Phys. Rev. Lett.* **10**, 159 (1963); J. Hubbard, *Proc. Roy. Soc. London* **A276**, 238 (1963).
12. J. B. Marston and I. Affleck, *Phys. Rev.* **B39**, 11538 (1989).
13. G. Czycholl and Q. Qin, *Phys. Rev. Lett.* **68**, 3244 (1992).
14. J. H. Samson, *Phys. Rev.* **B30**, 1437 (1984), *J. Magn. Magn. Mater.* **54-57**, 983 (1986).
15. A. V. Chubukov and K. A. Musaelian, *Phys. Rev.* **B50**, 6238 (1994).
16. A. Singh and E. Fradkin, *Phys. Rev.* **B35**, 6894 (1987); A. Singh, *Phys. Rev.* **B43**, 3617 (1991); P. K. Maiti and A. Singh, *Phys. Rev.* **B49**, 6078 (1994).
17. W. Nolting, A. Vega and T. Fauster, *Z. Phys.* **B96**, 357 (1995).
18. L. G. Yaffe, *Rev. Mod. Phys.* **54**, 407 (1982).
19. P. Coleman, *J. Magn. Magn. Mater.* **47-48**, 323 (1985).
20. M. Suzuki, *Commun. Math. Phys.* **51**, 183 (1976).
21. R. M. Wilcox, *J. Math. Phys.* **8**, 962 (1967) gives a number of useful results.

22. M. Suzuki, *Phys. Lett.* **A156**, 319 (1990), *Physica* **A194**, 432 (1993).

23. J. E. Hirsch, R. L Sugar, D. J. Scalapino and R. Blankenbecler, *Phys. Rev.* **B26**, 5033 (1982).

24. J. R. Klauder, *Phys. Rev.* **D19**, 2349 (1979).

25. E. Fradkin, *Field Theories of Condensed Matter Systems* (Addison Wesley, Redwood City, 1991).

26. E. Fradkin and M. Stone, *Phys. Rev.* **B38**, 7215 (1988).

27. H. Kuratsuji, *Phys. Rev. Lett.* **61**, 1687 (1988).

28. H. Takano, in Ref. 9, p.%44.

29. V. R. Vieira and P. D. Sacramento, *Physica* **A207**, 584 (1994).

30. A. Perelomov, *Generalized Coherent States and Their Applications* (Springer, Berlin, 1986).

31. J. R. Klauder, *Phys. Rev.* **D19**, 2349 (1979).

32. P. B. Wiegmann, *Phys. Rev. Lett.* **60**, 821 (1988).

33. E. O. Tüngler and T. Kopp, preprint cond-mat/9412092 (1995).

34. S. F. Edwards, *Proc. Roy. Soc. London Ser.* **A 232**, 371 (1955).

35. B. Mühlschlegel and H. Zittartz, *Z. Phys.* **175**, 553 (1963).

36. D. J. Amit, *Field Theory, the Renormalization Group, and Critical Phenomena* (McGraw Hill, New York, 1978).

37. G. Morandi, E. Galleani d'Agliano, F. Napoli and C. F. Ratto, *Adv. Phys.* **23**, 867 (1974).

38. D. R. Hamann and J. R. Schrieffer, in *Magnetism* vol. 5, ed. H. Suhl (Academic, New York, 1973), p 237.

39. J. A. Hertz, *Phys. Rev.* **B35**, 1165 (1976).

40. G. Sugiyama and S. E. Koonin, *Ann. Phys. (NY)* **168**, 1 (1986).

41. S. Sorella, S. Baroni, R. Car and M. Parrinello, *Europhys. Lett.* **8**, 663 (1989).

42. B. Mühlschlegel, unpublished lecture notes, University of Pennsylvania (1965).

43. W. E. Evenson, J. R. Schrieffer and S. Q. Wang, *J. Appl. Phys.* **41**, 1199 (1970).

44. M. V. You and V. Heine, *J. Phys. F: Met. Phys.* **12**, 177 (1982).

45. K. S. Chana, J. H. Samson, M. U. Luchini and V. Heine, *J. Phys.: Condens. Matter* **3**, 6455 (1991).

46. J. Hubbard, *Phys. Rev.* **B19**, 2626 (1979), *Phys. Rev.* **B20**, 4584 (1979).

47. H. Hasegawa, *J. Phys. Soc. Japan* **49**, 178 (1980).

48. Y. Kakehashi, *J. Phys. Soc. Japan* **50**, 1505 (1981).

49. J. H. Samson, *J. Physique (Paris)* **45**, 1675 (1984).

50. J. H. Samson, in *Quantum Monte Carlo Methods in Condensed Matter Physics*, ed. M.%Suzuki (World Scientific, Singapore, 1993), p 235.

51. D. M. Edwards and A. C. Hewson, *Rev. Mod. Phys.* **40**, 810 (1964); D. M. Edwards, *J. Phys.: Condens. Matter* **5**, 161 (1993).

52. S. Sarkar, *J. Phys.: Condens. Matter* **4**, 10003 (1992).

53. R. Blankenbecler, D. J. Scalapino and R. L. Sugar, *Phys. Rev.* **D24** 2278 (1981).

54. J. E. Hirsch, *Phys. Rev.* **B31**, 4403 (1985).

55. D. Sherrington, *J. Phys. C: Solid St. Phys.* **4**, 401 (1971).

56. See T. Moriya, *Spin Fluctuations in Itinerant Electron Magnetism* (Springer, Berlin, 1985) and references therein.

57. See, for example, C. Itzykson and J.-M. Drouffe, *Statistical Field Theory* (CUP, Cambridge, 1989) chapter 5.

58. I. M. Gel'fand and A. M. Yaglom, *J. Math. Phys.* **1**, 48 (1960).

59. P. de Vries, PhD thesis, Universiteit van Amsterdam (1991).

60. R. P. Feynman, in *Quantum Implications*, ed. B. J. Hiley and F. D. Peat, (Routledge, London, 1987) p235.

61. S. Sorella, *Int. J. Mod. Phys.* **B5**, 937 (1991).

62. S. R. White, D. J. Scalapino, R. L. Sugar, E. Y. Loh, J. E. Gubernatis and R. T. Scalettar, *Phys. Rev.* **B40**, 506 (1989).

63. S. F. Edwards, *Phil. Mag.* **4**, 1171 (1959).

64. P. L. Silvestrelli, S. Baroni and R. Car, *Phys. Rev. Lett.* **71**, 1148 (1993).

65. M. T. Wilson and B. L. Gyorffy, *J. Phys.: Condens. Matter*, in press (1995).

66. R. Micnas, *Physica* **98A**, 403 (1979).

67. S. Leibler and H. Orland, *Ann. Phys. (NY)* **132**, 277 (1981).

68. I. V. Kolokolov, *Ann. Phys. (NY)* **202**, 165 (1990).

69. D. R. Hamann, *Phys. Rev.* **B2**, 1373 (1970).

70. H. Keiter, *Phys. Rev.* **B2**, 3777 (1970).

71. C. A. Macêdo and M. D. Coutinho-Filho, *Phys. Rev.* **B43**, 13515 (1991).

72. D. J. Amit and H. Keiter, *J. Low Temp. Phys.* **11**, 603 (1973).

73. R. A. Bari, *Phys. Rev.* **B5**, 2736 (1972).

74. R. F. Hassing and D. M. Esterling, *Phys. Rev.* **B7**, 432 (1973).

75. J. E. Hirsch, *Phys. Rev.* **B28**, 4059 (1983).

76. G. M. Buendia, *Phys. Rev.* **B33**, 3519 (1986).

77. J. E. Hirsch, *Phys. Rev.* **B34**, 3216 (1986).

78. G. G. Batrouni and P. De Forcrand, *Phys. Rev.* **B48**, 589 (1993).

79. H. Q. Lin and J. E. Hirsch, *J. Appl. Phys.* **61**, 3706 (1987).

80. J. E. Hirsch, *Phys. Rev.* **B35**, 1851 (1987).

81. M. L. Lyra, M. D. Coutinho-Filho and A. M. Nemirovsky, *Phys. Rev.* **B48**, 3755 (1993).

82. T. Moriya and H. Hasegawa, *J. Phys. Soc. Japan* **48**, 1490 (1980).

83. M. Cyrot, *J. Magn. Magn. Mater.* **45**, 9 (1984).

84. K. S. Chana, PhD thesis, Loughborough University of Technology (1993).

85. R. E. Prange, in Ref. 2, p 69.

86. B. L. Gyorffy, A. J. Pindor, J. Staunton, G. M. Stocks and H. Winter, *J. Phys. F: Metal Phys.* **15**, 1337 (1985).

87. B. Mühlschlegel, *J. Math. Phys.* **3**, 522 (1962).

88. H-U. Everts, *Z. Phys.* **199**, 211 (1967).

89. G. G. Batrouni and R. T. Scalettar, *Phys. Rev.* **B42**, 2282 (1990).

90. R. Schumann and E. Heiner, *Phys. Lett.* **A134**, 202 (1988).

91. J. M. Deutsch, *Phys. Rev.* **E50**, 2411 (1994).

92. M. V. Berry, *Proc. Roy. Soc. Lond.* **A392**, 45 (1984).

93. J. W. Zwanziger, M. Koenig and A. Pines, *Annu. Rev. Phys. Chem.* **41**, 601 (1990).

94. Y. Aharonov and J. Anandan, *Phys. Rev. Lett.* **58**, 1593 (1987).

95. A. Bohm, L. J. Boya and B. Kendrick, *Phys. Rev.* **A43**, 1206 (1991).

96. J. H. Samson, *Phys. Rev.* **B47**, 3408 (1993).

97. H. Urbantke, *Am. J. Phys.* **59**, 503 (1991) gives a number of illustrations of the geometry here.

98. N. Mukunda and R. Simon, *Ann. Phys. (NY)* **228**, 205 (1993).

99. A. Angelucci and G. Jug, *Int. J. Mod. Phys.* **B3**, 1069 (1989); A. Angelucci, *Phys. Rev.* **B44**, 6849 (1991).

100. G. Dopf, A. Muramatsu and W. Hanke, *Europhys. Lett.* **17**, 559 (1992), *Int. J. Mod. Phys.* **3**, 79 (1992).

101. S. J. Sciutto, U. Marini Bettolo Marconi and R. Medina, *Physica* **A171**, 139 (1991).

102. J. H. Samson, *Phys. Rev.* **B51**, 223 (1995).

103. M. Hillery, R. F. O'Connell, M. O. Scully and E. P. Wigner, *Phys. Reports* **106**, 121 (1984).

104. O. K. Vorov, in *Topological Phases in Quantum Theory,* ed. B. Markovski and S. I. Vinitsky (World Scientific, Singapore, 1989) p. 112.

105. R. D. Richtmyer, *Principles of Advanced Mathematical Physics Volume I* (Springer, Berlin, 1978) chapter 12.

106. E. H. Loh Jr., J. E. Gubernatis, R. T. Scalettar, S. R. White, D. J. Scalapino and R. L. Sugar, *Phys. Rev.* **B41**, 9301 (1990).

107. D. Marx, S. Sengupta and P. Nielaba, *J. Chem. Phys.* **99**, 6031 (1993).

108. S. Fahy and D. R. Hamann, *Phys. Rev.* **B43**, 765 (1991).

109. S. Fahy, in *Quantum Monte Carlo Methods in Condensed Matter Physics*, ed. M. Suzuki (World Scientific, Singapore, 1993), p 285; D. R. Hamann and S. Fahy, *Phys. Rev.* **B47**, 1717 (1993).

110. A. Muramatsu, G. Zumbach and X. Zotos, *Int. J. Mod. Phys.* **C3**, 185 (1992).

111. J. E. Gubernatis and X. Y. Zhang, *Int. J. Mod. Phys.* **C5**, 599 (1994).

112. J. E. Hirsch, *Phys. Rev. Lett.* **51**, 1900 (1983).

113. S. R. White and J. W. Wilkins, *Phys. Rev.* **B37**, 5024 (1988).

114. S. Sorella, in *Quantum Monte Carlo Methods in Condensed Matter Physics*, ed. M. Suzuki (World Scientific, Singapore, 1993), p 265.

115. G. H. Lang, C. W. Johnson, S. E. Koonin and W. E. Ormand, *Phys. Rev.* **C48**, 1518 (1993); Y. Alhassid, D. J. Dean, S. E. Koonin, G. Lang and W. E. Ormand, *Phys. Rev. Lett.* **72**, 613 (1994).

116. M. V. Berry, *Physics Today* **43**(12), 34 (1990). See figures 5 and 6.

117. R. Englman, *The Jahn-Teller effect in molecules and crystals* (Wiley, New York, 1972).

118. H. C. Longuet-Higgins, *Adv. Spectroscopy* **2**, 429 (1961); G. Herzberg and H. C. Longuet-Higgins, *Discuss. Faraday Soc.* **35**, 77 (1963).

119. G. Delacrétaz, E. R. Grant, R. L. Whetten, L. Wöste and J. W. Zwanziger, *Phys. Rev. Lett.* **56**, 2598 (1986).

120. M. Takasu, S. Miyashita and M. Suzuki, in Ref. 9, p. 114.