It is a direct consequence of Perron's theorem that this eigenvector corresponds to the largest eigenvalue and is nondegenerate

Perron's theorem (see Goldenfeld (?.3))

The largest eigenvalue of a strictly positive matrix is:
a) real positive
b) non-degenerate
c) An analytic function of the m.e.
+ in Goldenfeld $\longrightarrow$ d) all component of the eigenvector are > 0

Corollary: An eigenvector of a real symmetric matrix with all components > 0 corresponds to the largest eigenvalue and is nondegenerate

proof: suppose that there is another eigenvector corresponding to the largest eigenvalue. Then it has all components > 0. For a real symmetric matrix, all eigenvectors are orthogonal, and two positive eigenvectors cannot be orthogonal.

For an ergodic Markov process all m.e. of a finite power of $T(c, c')$ and $R(c, c')$ are > 0.
We can apply Perron's theorem to this power of $R(c, c')$.
Of course, $R^p(c, c')$ and $R(c, c')$ have the same eigenvectors

We have to construct an algorithm that is ergodic and that satisfies detailed balance.

16d) Metropolis Algorithm

Transition probability

$$T(c,c') = 1 \quad \text{if} \quad \frac{e^{-\beta H(c')}}{e^{-\beta H(c)}} > 1$$

$$T(c,c') = \frac{e^{-\beta H(c')}}{e^{-\beta H(c)}} \quad \text{if} \quad \frac{e^{-\beta H(c')}}{e^{-\beta H(c)}} < 1$$

Metropolis satisfies detailed balance

$$\frac{T(c,c')}{T(c',c)} = \frac{1}{\left(e^{-\beta H(c)}/e^{-\beta H(c')}\right)} \quad \text{if} \quad \frac{e^{-\beta H(c')}}{e^{-\beta H(c)}} > 1$$

$$= \frac{e^{-\beta H(c)}}{e^{-\beta H(c')}} \quad \text{if} \quad \frac{e^{-\beta H(c')}}{e^{-\beta H(c)}} < 1$$

We choose δc such that the algorithm is ergodic

10e) Heat bath algorithm

This algorithm uses the exact probability distribution of the local integration variable.
The advantage is that we don't have to rely on asymptotic convergence.
The problem is that this algorithm is difficult to implement.

The transition probability is given by

$$T(c_i, c_i') = \frac{1}{Z_i}\, e^{-\beta H(c_i')}$$

$$Z_i = \sum_{c_i'} e^{-\beta H(c_i')}$$

detailed balance is trivially satisfied

$$e^{-\beta H(c)}\, T(c, c') = e^{-\beta H(c')}\, T(c', c)$$

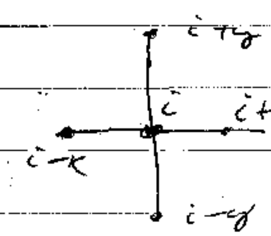
(c' differs from c by the update of one spin)

Example: Ising model in 2d

$$H(S') = k\left(S_i S_{i+x} + S_i S_{i-x} + S_i S_{i+y} + S_i S_{i-y}\right)$$

neighboring spins are fixed

then $$T(\underset{\text{contains } s_i}{c}, \underset{\text{contains } S_i'}{c'}) = \frac{e^{-\beta (H(S_i'))}}{\sum_{S_i'} e^{-\beta H(S_i')}}$$



16g) Fokker-Planck equation

Evolution of probability $P(q(\tau))$

Put $y = q(\tau_{n+1})$
$x = q(\tau_n)$

Then $$P(y, \tau_{n+1}) = \left\langle \int dx\, \delta\left(y - x + \frac{\partial S}{\partial q} d\tau - \eta'(\tau)\sqrt{d\tau}\right) \times P(x, \tau_n) \right\rangle_\eta$$

expand to 2^{nd} order in $d\tau$

$$P(y, \tau_{n+1}) = \int dx\, P(x, \tau_n) \Big(\delta(y-x) + \frac{\partial S}{\partial q} d\tau\, \delta'(y, x) - \eta'(\tau)\sqrt{d\tau}\, \delta'(y-x) + \frac{1}{2}\delta''(y-x)(\eta(\tau))^2 d\tau \Big\rangle$$

remove derivatives of δ-function by partial integration
$\langle \eta(\tau) \rangle = 0$

$$\Rightarrow P(y, \tau_{n+1}) = P(y, \tau_n) + \partial_y \left[P(y, \tau_n) \frac{\partial S}{\partial q_n} \right] \Delta t + \frac{\Delta t}{2}\, 2\, \partial_y^2\, P(y, \tau_n)$$

$\uparrow$ from average over η

Continuum limit $\Rightarrow$ $$\boxed{\partial_\tau P = \partial_y \left(P \frac{\partial S}{\partial y} \right) + \partial_y^2 P}$$

This is the Fokker-Planck equation

16f) Langevin equation

We wish to evaluate the integral

$$\langle F(q)\rangle = \int dq\, F(q)\, e^{-S(q)} \Big/ \int dq\, e^{-S(q)}$$

for example q is a continuous classical spin variable

idea: introduce a time variable τ such that $q(\tau)$ samples q-space according to $e^{-S(q)}$

This is achieved by the Langevin equation

$$\partial_\tau q = -\frac{\partial S}{\partial q} + \eta(\tau)$$

Gaussian noise term

$\langle \eta(\tau)\rangle = 0$
$\langle \eta(\tau)\,\eta(\tau')\rangle = 2\,\delta(\tau-\tau')$

Without noise $q(\tau)$ moves to the minimum of S

Discrete τ: $\tau = n\,\Delta t \quad \tau' = m\,\Delta t$

$$\langle \eta(\tau)\,\eta(\tau')\rangle = \frac{2\,\delta_{nm}}{\Delta t}$$

rescale $\eta'(\tau) = \sqrt{\Delta t}\,\eta(\tau) \Rightarrow \langle \eta'(\tau)\,\eta'(\tau')\rangle = 2\delta_{nm}$

Discrete evolution $q_{n+1} - q_n = -\frac{\partial S}{\partial q}\,\Delta t + \eta'(\tau)\sqrt{\Delta t}$