Licentiate Thesis

Astrophysical and Collider Signatures of Extra Dimensions

Henrik Melbéus

Theoretical Particle Physics, Department of Theoretical Physics,
School of Engineering Sciences
Royal Institute of Technology, SE-106 91 Stockholm, Sweden

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Cover illustration: A Feynman diagram contributing to the three leptons and large missing energy signal, in a model where right-handed neutrinos propagate in an extra dimension. Taken from Ref. [3].

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Abstract

2.3 The Metropolis Monte Carlo method The principle of importance sampling in statistical physics as suggested by Metropolis et al. [83] is as follows. In Fig. 2.1 we generated numbers x and from a uniform distribution. In the evaluation of something like (2.1), we could instead imagine generating the configurations $\mu \equiv \{\theta_i\}_{i=1}^{N}$ not uniformly, but in such a way that the number of hits and misses are roughly equal. The estimated expectation value after M generated configurations μ_n can be written

$$\langle O \rangle = \frac{\sum_{n=1}^{M} O_{\mu_n} e^{\beta H \mu_n}}{\sum_{n=1}^{M} e^{\beta H \mu_n}} \tag{1}$$

for states μ_n generated with uniform probability. If we instead were to draw configurations with probabilities according to their Boltzmann weights, the estimator is simply an unweighted arithmetic average

$$\langle O \rangle \approx \sum_{n=1}^{M} O_{\mu_n} \tag{2}$$

for states μ_n generated with probability $e^{-\beta \mu_n}$

The remaining question is then how one generates configurations with probability according to their Boltzmann weights. In practice, the importance sampling discussed above is obtained with a Markov chain through the Metropolis method [83]. Metropolis Monte Carlo works by proposing a new configuration j from an old configuration i with a proposal distribution $g(i \to j)$, which is accepted with a specified probability $A(i \to j) = min(1, e^{-\beta \Delta E})$ where $\Delta E = E_j - E_i$. Consider the time evolution of the probability of being in state i,

$$\frac{\mathrm{d}p_i}{\mathrm{d}t} = \sum_j [p_j P(j \to i) - p_i P(i \to j)] \tag{3}$$

where $P(i \to j)$ is the probability of transitioning from i to j. The first and second terms on the right-hand side correspond to the rate of transitioning into and out of the state i respectively. In equilibrium the time derivative is zero and (2.5) is fulfilled if (but not only if)

$$p_j P(j \to i) = p_i P(i \to j) \tag{4}$$

The condition of (2.6) is called detailed balance and is a sufficient but not necessary condition for Metropolis Monte Carlo given that states are generated ergodically, see [84, 88]. Ergodicity means that each state is reachable from every other state in a finite time, however a non-ergodic calculation may still yield useful information within an ergodic class [84]. In a simulation, the probability of transitioning from i to j is the product of the proposal and acceptance probabilities, that

is $P(i \to j) = g(i \to j)A(i \to j)$ which after insertion into the balance equation (2.6) gives

$$\frac{p_i}{p_j}\frac{g(j \to i)\min(1, e^{-\beta(E_i - E_j)})}{g(i \to j)\min(1, e^{-\beta(E_j - E_i)})} = \frac{e^{-\beta E_i}}{e^{-\beta E_j}} \tag{5}$$

assuming that the proposal distribution is symmetric. The Metropolis Monte Carlo method thus generates a chain of configurations where each configuration appears with a probability proportional to its Boltzmann weight. The estimation of thermal averages can thus be done via arithmetic averaging of the form (2.4) by starting with some initial configuration μ_0 and generating a chain $\mu_1, ..., \mu_M$ via the Metropolis scheme. 2.5 Phase transitions: definition and classification

The thermodynamical bulk free-energy density $f = \beta - 1\ln(Z)/V$ depends on the coupling parameters of the Hamiltonian, and thermodynamic functions are calculated via differentiation of the free energy. Such thermo-ynamic functions may exhibit discontinuities at certain sets of coupling parameters, for which the free energy is not analytic. Such sets can be taken as definitions of phase boundaries which separate phases (i.e. regions of analyticity). The crossing of a phase boundary is then understood as a phase transition. It should be noted that the definition in terms of analytic free-energy is not completely general, considering the BKT-transition. For further details of mathematical aspects of phase transitions, we refer to [94] and for a more physical discussion to [95].

By the Ehrenfest classification [96] phase transitions are classified by the order of the derivative of the free energy which has a discontinuity at the critical point. If a first order derivative (e.g. entropy, internal energy) is discontinuous, then the phase transition is of first order. If a second order derivative (e.g. heat capacity) is discontinuous, the phase transition is of second order, and so on.

The Ehrenfest classification is however discouraged [95, 98], for example there may be divergences rather than dis- continuities in thermodynamic functions (as for the 2D Ising model without external field, where the heat capacity diverges logarithmically at T_c). The modern classification of phase transitions is binary where a phase transition is either 'first-order' (there is a latent heat for a temperature-driven transition) or âcontinuousâ (no latent heat) [98, 95].

Preface

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