Macroscopic Interpretation of Microscopic models

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Abstract

The method of renormalization group and its associated geometric language for describing macroscopic phenomenology is a powerful technique for studying physics problems with many degrees of freedom. The abstract problem solving strategy embodied by the method – solving a hard problem by transforming it to a sequence of similar but simpler problems – acquires new power in the context of sophisticated physical theories. This paper describes a procedural implementation of the idea and suggests new research problems to turn this powerful technique into a qualitative reasoning method.

Introduction

Model interpretation – extracting useful consequences out of a mathematical model – is a key problem in many areas of science and engineering. So it is not surprising that many qualitative reasoning research efforts are devoted to this task. Causal and incremental analysis of devices [de Kleer, 1984; Williams, 1984; Weld, 1988], envisionment and qualitative simulation of qualitative equations [Forbus, 1984; Kuipers, 1986], dimensional and order of magnitude analysis of algebraic and differential equations [Bhaskar and Nigam, 1990; Mavrovouniotis and Stephanopoulos, 1988; Raiman, 1991; Yip, 1993], and phase space analysis of dynamical systems [Sacks, 1991; Yip, 1991; Zhao, 1991; Nishida *et al.*, 1991; Bradley and Zhao, 1993] – these machineries have found applications in many domains.

Interpretation problems can be characterized according to three dimensions: (1) the essential degrees of freedom in the system (or roughly its size), [1] (2) the kind of information given as input, and (3) the kind of information required as output. In general, the difficulty of analysis increases rapidly as the degrees of freedom or the uncertainty of the input or the demand for precision of the output increase.

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[1] Essential degrees of freedom measures the extent to which the parts of the systems are essentially coupled.

So far there has not been much attention paid to systems with many (or practically infinite) degrees of freedom. Many problems in physics have this character: phase transition of fluids, spontaneous magnetization of ferromagnetic material, and effective transport in turbulence, just to name a few. Common among these problems is the task of extracting macroscopic or large-scale behaviors of a system from its microscopic properties. It is not immediately obvious how the extraction can be done because neither direct numerical simulation nor analytical solutions of equations involving a huge number (could be on the order of 10^{23}) of interacting variables is feasible.

A macroscopic description is possible whenever the nitty-gritty of the microphysics can be subsumed into a few phenomenological parameters. Water, oil, or gas are complicated systems made up zillions tiny molecules interacting with some complicated force laws. However, their macroscopic properties can be summarized by similar functional relationships among few material constants like density and viscosity. The functional relationship is usually universal for a large class of fluids, while the specific values of the material constants are the detail-sensitive parts.

About twenty years ago Ken Wilson invented a technique known as the renormalization group (RNG), which becomes a standard method for constructing macroscopic theories from microscopic models [Wilson, 1975]; he was awarded a Nobel prize for this work. The technique has been applied in many areas other than critical phenomena, and continues to be a subject of current research. The purpose of this paper is two-fold: (1) to give an elementary description of the RNG method in terms of procedures, and (2) to suggest problem areas that might be fruitful to work on from the qualitative reasoning perspective.

There are several reasons why we propose to study RNG. First, RNG is based on a surprisingly simple idea: one solves a hard problem by transforming it to a similar but simpler one with the same answer, and by iterating the transformation until one arrives at a problem that is almost trivial to solve. Second, viewed as an abstract problem solving strategy, RNG is noth-

ing novel. The method acquires new power when it is combined with problem-specific knowledge structures. Isolating the essence of the method and understanding its scope might provide a new source of problems for investigation into the fundamental issues of descriptive language, styles of reasoning, and representation techniques in qualitative reasoning. Third, explicit procedural encoding of RNG has an educational benefit: it might provide a better medium for beginners to learn and use this technique. Fourth, RNG has solved some of the hardest problems in physics, and theoretical scientists are applying it to all sorts of problems: percolation, onset of superfluidity, polymer conformation, elementary particle excitation, and turbulence, just to take a few examples [Wilson, 1983]. Therefore, automating aspects of the RNG will likely have a large payoff.

Despite the appearance of automating a technique applicable to a specialized class of problems, we want to stress our more general concerns for this line of research:

- To study the nature of scientific reasoning as practiced in normal science. We would like to codify some of the skills that professionals have in formulating problems, making approximations, explaining data, and testing theories.
- To solve real problems in an area of significance to modern science.
- To provide scientists with an intelligent workbench consisting of a library of powerful heuristic and qualitative methods.

The paper is organized as follows. We begin by describing the task of extracting macroscopic properties. Next we explain intuitively how and why the RNG works. Then we illustrate the procedural implementation of a particular type of RNG method. Finally, we conclude with problem areas that might need most "cognitive" help.

The task: extracting macroscopic behaviors

Given a microscopic model with many degrees of freedom, the goal is to predict macroscopic behaviors that are independent of the inessential details of the microscopic model. This task is in general very difficult. The first difficulty is the large number of interacting variables; the second is that one does not really know which aspects of the microscopic model are inessential until one has solved the problem.

As an illustration of this task, we will consider a theoretical model for the spontaneous magnetization of ferromagnetic material. The theoretical model is known as the two-dimensional Ising model, one of the rare statistical mechanics models that can be solved exactly [Onsager, 1944]. Its study is still of considerable interest for two reasons: (1) it is probably the simplest nontrivial problem to illustrate the essence of RNG, and (2) many variants of the model, such as the 3D Ising model, useful for the study of other critical phenomena cannot be solved explicitly, but RNG is still applicable to them.

At room temperature a piece of iron is ferromagnetic. At the microscopic level, the iron can be thought of as consisting of many tiny little atomic magnets spinning perpetually. The interaction forces among them are such that at low temperature two neighboring magnets tend to align in the same direction: both up or both down. As a result many more magnets will point to one direction than any other direction, creating a net magnetization at the macroscopic level. Thus, the piece of iron behaves like a bar magnetic. If the iron is heated, the atomic magnets will flip randomly due to the increasing thermal energy, and the alignment will be disturbed. At a critical temperature, known as the Curie temperature (770 C), the net magnetization vanishes. The critical temperature marks the transition of the iron from the ferromagnetic to paramagnetic phase.

The net magnetization M, which for our purpose can be defined as the absolute value of the average excess of atomic magnets pointing up over down, is found to obey a power law:

$$M \quad \begin{cases} \propto & \mid T - T_c \mid^{\beta} \quad T < T_c \\ = & 0 \qquad\qquad T > T_C \end{cases}$$

where T_c is the critical temperature, and β is called a critical exponent. Experiments have found β to be approximately 0.12 for two dimensional ferromagnetic systems (Fig. 1). It is conveniently to rewrite the power law in terms of a dimensionless temperature called the reduced temperature defined by $t = \frac{T - T_c}{T_c}$: $M \propto \mid t \mid^{\beta}$. The quantity M is also called an **order parameter** because it signifies the degree of orderliness of the system. At zero temperature the order parameter attains its maximum value.

A second important phenomenological quantity is the **correlation length**, which measures the maximum range of distance over which fluctuations in one part of the system (say the flipping of a magnetic spin) are correlated or have influence on fluctuations on another part of the system. When the correlation length is small, say on the order of a few separation distance of the atomic magnets, the system can be partitioned into a large number of statistically independent cells. As the critical point is approached, the correlation length grows rapidly and it eventually becomes comparable to the size of the system. Experiments have found the correlation length, denoted by ξ, *diverges* near the critical temperature and obeys the power law:

$$\xi \propto \mid t \mid^{-\nu}$$

where the critical exponent ν is approximately 1 for two dimensional systems.

One reason why the critical exponents are significant is that they seem to be universal, i.e., they are

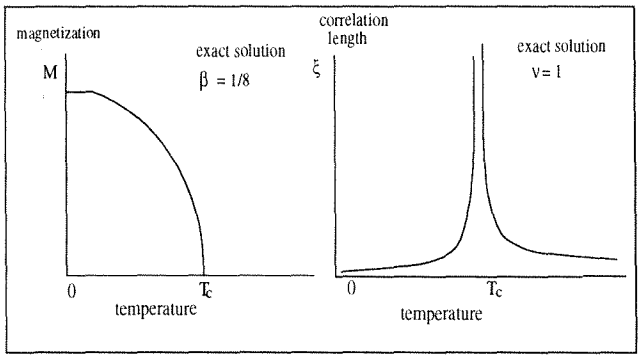

Figure 1: Schematic diagrams for the critical behaviors of the magnetization M and correlation length ξ for the 2D Ising model. For 3D Ising model, no exact solutions have been found; experimental data suggest $\beta \approx 0.33$ and $\nu \approx 0.63$.

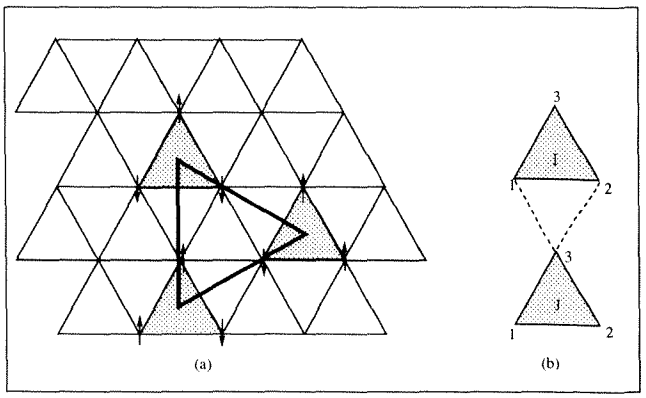

Figure 2: (a) Ising model defined on an infinite triangular lattice. Each site spins can point either up or down. Nine of them are shown. A block spin is formed by grouping three site spins within a shaded triangle. The value of a block spin is determined by a majority rule. The block spins form a coarse-grained system which is a scaled version of the original one. (b) Neighboring block spins can interact via two ways in the first order calculation. The interactions are indicated by dashed lines.

remarkably insensitive to the microscopic details of the system. A whole range of fluids and magnets have exponents that fall in a narrow range of the β and ν values. The coincidence is particularly impressive when the critical exponents are not simple fractions like $\frac{1}{2}$ or $\frac{1}{3}$; some of them are believed to be irrational numbers. That means simple dimensional analysis will give *wrong* answers to the exponents.

The question of interest is: *Can the values of the critical exponents β and ν be predicted from a microscopic description in terms of atomic magnets?*

Let's describe what input is required for the calculation. The input is a microscopic model with many degrees of freedom. Three ingredients are needed: (1) the microscopic variables and the values they can take, (2) a description of how the microscopic variables interact, and (3) a prescription for calculating averages.

Let's see what these ingredients are in the context of the 2D Ising model. Imagine a triangular lattice of spins (Fig. 2a), each of which can take one of the two values: +1 or -1. Physically it means the spins are constrained to point either in the up or down direction. The N spins, where N is of $O(10^{23})$, define 2^N possible configurations for the system.

Each spin interacts with its nearest neighbors in such a way the interaction energy is lowered if the spins are aligned in the same direction: both up or both down. Mathematically the interaction can be described by a Hamiltonian H:

$$H = -K \sum_{<i,j>} s_i s_j$$

where $K > 0$ is the **coupling constant**, measuring the interaction strength between the nearest-neighbors s_i and s_j. One could complicate the model by adding an external field, triple interactions, quadruple interactions, and so forth. Physically, the Hamiltonian defines the total energy of a particular configuration. Because nature favors lower energy states, we put the negative sign in front of K so that the lowest energy states correspond to the configurations in which all the spins are perfectly aligned: all up (+1) or all down (-1).

To define the averaging operator, we appeal to a fundamental result in statistical mechanics, namely, the probability p_s of a configuration s with Hamiltonian H_s is given by:

$$p_s = \frac{e^{-\frac{H_s}{k_B T}}}{Z}$$

where k_B is the Boltzmann constant, T the temperature, and Z the partition function defined by:

$$Z = \sum_s e^{-H_s}$$

where the sum is taken over all possible configurations s. It is conventional to absorb the factor $\frac{1}{k_B T}$ into the coupling constant K. The inverse dependence on temperature means that as the temperature is raised, the coupling strength will decrease, thereby increasing the tendency of spins to misalign.

The average of a quantity A is defined as the configuration sum weighed by the Boltzmann probability p_s:

$$< A >= \sum_s A_s p_s$$

where A_s is the value of A in a configuration s.

Renormalization Group: a method and a new language

The universality of the critical exponents has an important consequence. Since the exponents are universal, it

is almost tautological to assert that they do not depend on the microscopic details. And therefore the critical exponents will be invariant under any transformation of the system that removes the details but preserves large-scale behaviors. We'll be more precise with this statement shortly.

The central idea of RNG is the iterative removal of degrees of freedom from the microscopic model in such a way that at every stage the new system we get is similar to the old one we start with. Consider a portion of the infinite triangular lattice with nine spins (Fig. 2a). Instead of keeping track of all the individual spins, we might group the spins into blocks of three and represent the entire block by a single new spin whose value is determined only by the spins inside the block. For instance, the value of the new spin, called it a **block spin**, can be decided by a majority rule: if two or more of the spins inside the block are up (+1), then the block spin is up (+1); otherwise it is down (-1).

Notice the effect of the projection. The new system looks exactly like the old one – well not exactly because the coupling constant will in general be changed and new coupling constants for triple or higher order interactions might be introduced. Let us write the transformation of the old to new system symbolically as:

$$K' = R(K)$$

where the prime denotes the coupling constant for the new system. To anticipate the generation of new coupling constants, one usually starts with a more elaborate Hamiltonian with a set of coupling constants $K_1 \ldots K_n$ most of which are set to zero initially. The transformation R is called the **renormalization group transformation**. It is a renormalization because we expect the transformation to change only the values of the coupling constants – they are said to be renormalized – and not the structure of interaction. It is a group (in fact only a semi-group) because the transformation can be iterated but the inverse of the transformation is not well-defined as information is lost by the projection procedure.

The transformation has to satisfy one important constraint, namely, it must preserve the partition function of the system:

$$\sum_{s'} e^{-H_{s'}'} = \sum_{s} e^{-H_s}$$

where the sum on the left-hand side extends over the possible configuration s' of the block spins, and the sum on the right-hand side the possible configurations s of the original site spins.

With the projection and the requirement that the partition function be invariant, the transformation achieves the two basic goals of RNG: (1) to reduce the degrees of freedom (by a factor of 3 per iteration for this particular projection), and (2) to ensure the macroscopic quantities calculated from the new system are the same as those from the old one.

The significance of the transformation is revealed when we show that the critical exponents are calculable from the properties of the transformation equation. The first point to note is that the transformation R increases the lattice spacing by a factor of l ($l = \sqrt{3}$ in our example) per iteration, thereby *reducing* the correlation length ξ by the same factor in units of the original microscopic lattice spacing. For almost all values of K, if the transformation is iterated infinitely many times, the correlation length will be reduced to zero. This reduction will occur except at a value of K where the correlation length is infinite to begin with, i.e., at a K value corresponding to the system's critical temperature. Physically it means that a system starts off with a critical temperature will remain at the critical temperature under the transformation. At all other temperature – no matter how close it is to the critical temperature – the system will be driven away from its critical state.

This last observation points to the importance of the unstable fixed point of the transformation equation: it corresponds to the system at its critical temperature and therefore the critical exponents should be calculable from properties of the unstable fixed point.

Fixed points of the equations are determined by the equation:

$$K = R(K)$$

Since R is in general a nonlinear mapping, there may be one or more fixed points. [2] The stability of a fixed point K^* is determined by the value of the derivative [3] of the mapping R with respect to K evaluated at the fixed point:

$$\lambda_t = \left.\frac{dR(K)}{dK}\right|_{K=K^*}$$

where λ_t is the eigenvalue; the subscript t indicates it is related to temperature. If λ_t is known, then the critical exponent ν can be calculated by (see Appendix A):

$$\nu = \frac{\log l}{\log \lambda_t}$$

where l is the factor by which length scale changes under the transformation.

A fixed point is physically significant because the system at its fixed point is **scale-invariant**, i.e, the correlation length is either 0 or ∞. A fixed point is called **trivial** if it corresponds to zero correlation length, and called **critical** if the correlation length is infinite.

More significant than the calculation of critical exponents is the fact that the geometry around a critical fixed point explains **universality**: it explains why different physical systems near its critical point have the

[2] Of course, the equation might not have any fixed point at all. In fact it is an open question to decide when a renormalization equation can have a fixed point.

[3] Or the Jacobian if K is a set of couple constants.

same behavior. To understand this, we exploit an analogy with dynamical systems. We first note that the set of coupling constants (say, $K_1, K_2, \ldots K_n$) of the Hamiltonian defines a n-dimensional K-space, called the **coupling space**. Each point in the K-space represents a physical system defined by the Hamiltonian with the values of K's at that point. The iterated action of the transformation R generates an orbit of points in the K-space. The simplest limiting behavior of the orbit is towards a fixed point. The basin of attraction of a fixed point defines a class of systems whose large-scale behaviors are determined by the geometry of orbits around that fixed point.

Consider as an example an Ising model with three coupling constants (K_1, K_2, and K_3). If it turns out that near a critical fixed point, the two directions K_2 and K_3 are contracting towards the fixed point, then these two coupling constants are called **irrelevant** because regardless of their initial values they tend to 0 under the action of R. In other words, at the critical fixed point, the system acts as if the irrelevant coupling constants don't exist.

Procedural implementation of a renormalization group method

In the previous section, we explain the significance of the renormalization group equation $K' = R(K)$. In particular, its critical fixed point determines the critical behaviors of the system. The heart of a RNG calculation is to find an explicit form for the transformation R, which except in a few rare cases cannot be calculated exactly. In the following we will explain the details of an implementation of a particular RNG method, the so-called real-space renormalization. An RNG calculation consists of 5 steps:

1. formulation of the microscopic model
2. projection
3. derivation of the transformation equation
4. solution of the fixed point equation
5. calculation of eigenvalues and critical exponents

Formulation of the microscopic model

Formulation of a novel problem within the RNG framework is arguably the most difficult step; it requires knowledge of the underlying physics of the problem and an articulation of what macroscopic properties one can reasonably expect RNG to be able to calculate. Applying RNG to problems in fully developed turbulence is a good illustration of the kind of difficulties one typically encounters [Yakhot and Orszag, 1986].

Fortunately the theoretical frameworks for studying a large class of problems in statistical mechanics (and quantum field theory) are already in a form amendable to RNG analysis. The Hamiltonian is represented by a higher-order procedure of two arguments, configuration and K. Representing objects like hamiltonian or configuration as procedures has two advantages: (1) the object can be manipulated by algebraic operations, and (2) the object can be evaluated to give numbers.

```
(define hamiltonian
  (lambda (configuration K)
    (mult -1
          (mult K
                (sum (lambda (i j)
                       (mult (configuration i)
                             (configuration j)))
                     nearest-neighbor?
                     (pick-2-combinations
                       (configuration 'names)))))))
```

We have used a few auxiliary procedures in the definition of the hamiltonian. The **mult** procedure is a generic multiplication, handling both numbers and algebraic expressions. The **sum** procedure takes three arguments: (1) a term to be summed over, which is itself a procedure taking n indices (2) a filter predicate, which removes indices not satisfying the predicate, and (3) the set of all indices. In the example, **nearest-neighbor?** is the filter predicate; it returns true if two site indices are nearest neighbors. The expression **(configuration 'name)** gives all site labels, and the procedure **pick-2-combinations** returns all possible pairs of site labels.

The partition function is represented by:

```
(define partition-function
  (lambda (hamiltonian coupling-constant configs)
    (sum (lambda(config)
           (exp* (mult -1 (hamiltonian
                           config
                           coupling-constant))))
         identity
         configs)))
```

The **exp*** is a generic exponentiation procedure.

Projection

This step is the projection or coarse-graining of the system: the grouping of spins into blocks. The purpose of coarse-graining is to reduce the original problem to a problem with fewer degrees of freedom. Many choices of projection are possible, and each choice determines a renormalization transformation. Some choices just affect the ease of calculation, while others might produce transformations that either have no fixed point or generate non-physical fixed points. Although no sufficient condition on the validity of a projection operator has been proven, several necessary conditions are known. The most important requirement is that the coarse-grained system must be similar to the microscopic system, which means symmetry of the system is preserved under the projection. For instance, a projection that changes the dimension of the system or maps a scalar spin variable to a vector will certainly produce spurious results.

The majority rule described in previous section works very well with 2D Ising models. The value of

a triangular block spin is +1 when two or more of its spins are +1, and is -1 otherwise.

Derivation of the renormalization equation

The constraint that the partition function be invariant relates the coarse-grained and the original Hamiltonian (see Appendix B):

$$-H'(S) = \log Z_0 + < V >_0$$

where Z_0 represents the energy contributed by *intra-block* spin interactions, while $< V >_0$ is the first term in the approximation for the energy contributed by *inter-block* spin interactions (Fig. 2b). The term $\log Z_0$ can be ignored in the calculation of critical exponents because the term is analytic and contains no singularities [Goldenfeld, 1992].

In the second term on the right-hand side, the subscript 0 in the average operator indicates that the average is partial: the sum extends over the local site configurations inside one block as opposed to over the entire block configuration. Physically, it means the effect of the smaller site spins is averaged out during the coarse-graining operation.

The partial average operator has nice properties:

1. it is linear, i.e., $< A+B >_0 = < A >_0 + < B >_0$ and $< cA >_0 = c < A >_0$ where c is a constant,
2. it is separable, i.e., $< AB >_0 = < A >_0 < B >_0$ if A and B belong to separate blocks,
3. it is symmetrical with respect to site spins, i.e., $< s_i >_0 = < s_j >_0$ if for any two site spins s_i and s_j belonging to the same block.

These rules allow the expression for V to be simplified. The end result is (Appendix C):

$$< V >_0 = 2K(\frac{e^{3K} + e^{-K}}{e^{3K} + 3e^{-K}})^2 \sum_{<IJ>} S^I S^J$$

Comparison with the form of the coarse-grained Hamiltonian:

$$H'(S) = -K' \sum_{<IJ>} S^I S^J$$

yields the renormalization equation:

$$K' = 2K(\frac{e^{3K} + e^{-K}}{e^{3K} + 3e^{-K}})^2$$

The algebraic simplifier to evaluate these expressions has two parts: (1) a set of rewrite rules incorporating the properties of the partial average operator, and (2) explicit calculation of the partial average for spin variables.

Solution of the fixed point equation

To find the fixed point, we just use the Newton's method:

```
> (newton
    (lambda(k)
      (- k
         (* 2
            (* k
               (* (^ (+ (EXP (* -1 K)) (EXP (* 3 K)))
                     2)
                  (^ (+ (* 3 (EXP (* -1 K)))
                        (EXP (* 3 K))) -2)))))))
  1)

0.3356134
```

An arbitrary initial guess 1 is used. The answer 0.336 compares reasonably well to the exact value $K_c = 0.275$.

Calculation of the critical exponents

The derivative is done symbolically and then numerically evaluated at the fixed point to get λ_t. The correlation length exponent ν follows from the formula: $\nu = \frac{\log l}{\log \lambda_t}$, where $l = \sqrt{3}$. The answer 1.133 is reasonably close to the exact value 1.

Calculation of the magnetization exponent β requires the addition of an external field to the starting Hamiltonian. The algebra with two coupling constants is little more complicated, but no new idea is involved.

Evaluation

How good is the block spin renormalization?
The method carried to first order gives reasonable estimates for critical K_c and the correlation length ν. But the estimate for β is not as good; it in fact gets the wrong sign. When the calculation is carried to second order, we get big improvements: within one percent accuracy for β and four percent for ν. But the approximation seems to be asymptotic at best because third order calculations give *worse* answer.

The last conclusion seems to be generally true for real-space renormalization methods. The reason appears to be the uncontrolled proliferation of new coupling constants as the calculation is carried to higher order. More accurate renormalization methods are available: for dimension greater than two, the Fourier-space (or momentum-space) ϵ expansion [Goldenfeld, 1992] is most accurate, while for dimension two or less, the Monte Carlo renormalization method seems most promising [Swendson, 1979].

Despite the accuracy problem, the block spin renormalization is simple to understand and relatively easy to carry out. So whenever applicable it is still the first method to try in order to develop a qualitative feel for the problem.

How general is the procedural implementation?
The basic steps of RNG are very much the same for real-space and momentum-space methods. In the momentum-space method, integrals replace discrete partition sums. The projection operator is simpler: at

each stage fluctuations higher then certain cutoff frequencies are averaged out. But the partial averaging is harder: the integrals get complicated quickly. Formal diagrammatic methods like Feynman diagrams are often used to simplify the calculation of these integrals.

The implementation assumes the microscopic interactions are given by a Hamiltonian and the transformation invariant is the partition function. These assumptions limit its applicability to problems like turbulent transport which has no Hamiltonian formulation and is far away from equilibrium. Generalizing RNG analysis beyond the equilibrium statistical mechanics formulation is an active research area in physics.

Three open problems to explore

"Where the renormalization group approach has been successful, a lot of ingenuity has been required: one cannot write a renormalization group cookbook."
— Ken Wilson, 1975.

Even within the realm of classical real-space and momentum space renormalization methods, there are still many areas that would benefit from computer help. By computer help, I don't mean numerical methods nor algebraic manipulations. Rather I mean cognitive help to aid a scientist in making judicious choice of the projection operator, the systematic exploration of the coupling space, and strategic formulation of the microscopic model.

Intelligent choice of projection operator

The projection operator and the order parameter for the ferromagnetic Ising model are easy to construct because the ground states are extremely simple: all spins up or all spins down. For most other cases, the choice is not obvious. I will give two examples.

The antiferromagnetic Ising model [Creswick, 1992] is identical to the ferromagnetic one except the nearest-neighbor coupling constant K is *negative*. Physically, it corresponds to a situation in which the tiny atomic magnets prefer to be antiparallel to each other. Inside a triangular block of three spins, at least one of the bonds will be frustrated because there is no way to arrange the three spins so that they are all antiparallel to each other. A blind application of the 3-spin majority rule will lead to totally wrong answer.

The second example is the so-called XY-model [Creswick, 1992], a generalization of the 2D Ising model where the spins can point to any direction on a plane – like a compass needle. The model is proposed as a theoretical model to study the behavior of superfluid He^4. Again a naive application of the majority rule gives disastrous results. It turns out that the ground states contain "vortices" and the easiest way to deal with them is by a momentum-space type integration done in the real space.

These two examples are fairly typical. The failure of a projection operator can usually be traced to the misidentification of the ground states and the violation of the symmetry group of the ground states. The open problem is: *Is there a general rule to construct a projection operator that will respect the symmetry group of the given ground states?*

Systematic exploration of the coupling space

The geometry of orbits in the K-space contains information not only about critical behaviors but also about non-critical macroscopic properties over the entire phase diagram (e.g., the liquid-gas first order transition). The open problem is: *Can the fixed points of an RNG transformation and their connection in the K-space be mapped out intelligently?* This problem is reminiscent of the qualitative reasoning research in automatic phase space analysis.

Strategic formulation of the microscopic model

Many physics problems have no obvious Hamiltonian formulation. The open problem is: *Is there a general characterization of the basic ingredients necessary for the application of RNG?* After all the twin principles of RNG – the systematic removal of degrees of freedom and the preservation of large-scale behaviors – do not seem to depend on the Hamiltonian formulation.

Conclusion

In this paper, I have explained the essence of RNG, illustrated the procedural implementation of a particular real-space renormalization method, and proposed some open problems for qualitative reasoning research. The interest in RNG lies not so much in the calculation of critical exponents but in its methodology to extract macroscopic properties from microscopic descriptions without explicitly solving a huge number of coupled equations. Covering a qualitatively new class of problems, RNG could be a welcome addition to the qualitative reasoning arsenal. The abstract problem solving strategy that RNG embodies – solving a hard problem by reducing it to a sequence of similar but simpler problems – acquires new power in the context of sophisticated physical theories. Without the guide of problem-specific knowledge, the method remains sterile. Articulation of these specific knowledge structures and use of them to guide the application and interpret the results of RNG methods – these two tasks might hold the key to helping scientists solve some of the hardest problems in science.

Appendix A: Calculation of critical exponent ν

Let K_c be the critical fixed point of the RNG equation and K' near K_c.

$$\begin{aligned} K_c = R(K_c) \quad &\Rightarrow \quad K' - K_c = K' - R(K_c) \\ &\Rightarrow \quad K' - K_c = R(K) - R(K_c) \\ &\Rightarrow \quad K' - K_c = \lambda_t (K - K_c) + O((K - K_c)^2) \\ &\Rightarrow \quad K' - K_c = l^{y_t} (K - K_c) \end{aligned}$$

But $\xi(K) = l\xi(K')$. Substituting the above result, we get $\xi(K - K_c) = l\xi(l^{y_t}(K - K_c))$. Since $\xi \sim \mid K - K_c \mid^{-\nu}$, we finally get $\nu = \frac{1}{y_t} = \frac{\log l}{\log \lambda_t}$.

Appendix B: Calculation of the transformation invariant

The transformation must preserve the partition function:

$$\sum_{s'} e^{-H'_{s'}} = \sum_{s} e^{-H_s}$$

Rewrite the sum on the left on right-hand side as a double sum: first sum over the site configuration $\{\sigma\}$ consistent with a given block spin configuration s' and then sum over all block spin configurations. We get:

$$\sum_{s'} e^{-H'_{s'}} = \sum_{s'} \sum_{\sigma} e^{-H_{s',\sigma}}$$

which gives

$$e^{-H'_{s'}} = \sum_{\sigma} e^{-H_{s',\sigma}}$$

Write the Hamiltonian H in terms of two parts:

$$H = H_0 - V$$

where H_0 is the intra-block interaction, and V is the inter-block interaction. The negative sign in front of V simplifies some algebra. Then,

$$e^{-H'_{s'}} = \sum_{\sigma} e^{-H_{s',\sigma}} = \sum_{\sigma} e^{-(H_0 - V)} = Z_0 < e^V >_0$$

where $Z_0 \equiv \sum_{\sigma} e^{-H_0}$ and $< e^V >_0 \equiv \frac{\sum_{\sigma} e^{-H_0} e^V}{Z_0}$. Finally, take logarithm on both sides of the equation and keep the first term in the cumulant expansion [Goldenfeld, 1992, Chap 9]:

$$\log(< e^V >_0) = < V >_0 + O(V^2)$$

we arrive at: $-H' = \log Z_0 + < V >_0$.

Appendix C: Calculation of inter-block spin interactions

Write the inter-block spin interaction V as a sum of nearest-neighbor block interaction:

$$V = \sum_{<I,J>} V_{IJ}$$

Then

$$< V >_0 = \sum_{<I,J>} < V_{IJ} >_0$$

The partial average of V_{IJ} can be calculated as follows (Fig. 2b):

$$< V_{IJ} >_0 = < K S_3^J (S_1^I + S_2^I) >_0 = 2K < S_3^J >_0 < S_1^I >_0$$

where S_3^J denotes the site spin 3 insider block spin S^J. The partial average of a site spin is given by:

$$< S_1^I >_0 = \frac{e^{3K} + e^{-K}}{e^{3K} + 3e^{-K}} S^I$$

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