Zeitschrift: Helvetica Physica Acta
Band: 65 (1992)
Heft: 2-3

Artikel: Quantum Monte Carlo simulations : algorithms, limitations and applications
Autor: Raedt, H. de
DOI: https://doi.org/10.5169/seals-116407

Quantum Monte Carlo Simulations: Algorithms, Limitations and Applications

H. De Raedt
University of Groningen
NL 9700 AV Groningen, The Netherlands

Abstract. A survey is given of Quantum Monte Carlo methods currently used to simulate quantum lattice models. The formalisms employed to construct the simulation algorithms are sketched. The origin of fundamental (minus sign) problems which limit the applicability of the Quantum Monte Carlo approach is shown to be a generic feature of the formalisms used to devise the simulation algorithms. A brief overview of recent new developments is given.

Introduction

The discovery of high T_c materials has increased the interest in applying Monte Carlo methods to quantum many-body lattice problems. For an extensive review see [1]. The two most prominent models are the two-dimensional (2D) Hubbard model and S=1/2 Heisenberg model. In the strong-coupling limit and for a half-filled band, the former reduces to latter [2]. Away from half-filling but in the strong-coupling limit, the Hubbard model can be approximated by the $t-J$ model [3]. Within the context of high temperature superconductivity it is more appropiate to study an extension of the Hubbard model namely the Emery model [4]. For a review of recent developments on the (extended) Hubbard models see [5,6].

The fact that the 2D (and 3D) Hubbard model has defied accurate determination of various physical quantities suggests that computer simulation might be an alternative approach to gain insight into the behavior of one of the simplest models for describing strongly correlated electrons. However it turns out that the construction of such simulation algorithms pose great challenges as a number of conceptual and technical problems appear which apparently are difficult to overcome. Also in this respect the single-band Hubbard model can be considered as the simplest model offering the full spectrum of computational difficulties. With this in mind I will, in what follows, discuss various aspects of Quantum Monte Carlo techniques for lattice systems by using the single-band Hubbard model as the example. Generalizations to other fermionic systems such as extended Hubbard models [7-13] or the Anderson impurity model [14-18] are usually straightforward although the practical realizations are not.

Algorithms

Numerical investigations of models of interacting fermions employ either standard diagonalization techniques or combine the Trotter-Suzuki (path integral) formula and the Metropolis Monte Carlo (MMC) or Molecular Dynamics (MD) technique to simulate the system. The former approach yields numerically exact results for the ground state and, in those cases where all eigenvalues can be obtained, the thermodynamic properties. The applicability of the diagonalization technique is limited by the fact that it requires storage for at least two wave functions. These wavefunctions are represented as linear combinations of basis states, the number of which grows very fast with the system size. For instance the number of states of a half-filled 4×4 lattice system is approximately 16×10^7, disregarding reductions due to the use of symmetry. On the other hand it is extremely valuable as it is the only method capable of generating numerically exact results which other, less accurate, techniques need to reproduce before they can be applied to larger systems with some confidence.

In the simulation approach the quantum statistical problem involving very large matrices is replaced by a multi-dimensional sum. Techniques based on these ideas include Variational Quantum Monte Carlo (VQCM) [19], Green Function Monte Carlo (GFMC) [1,20], finite temperature Quantum Monte Carlo (FTQMC) [1,21], Projector Quantum Monte Carlo (PQMC) [1,21]. If the integrand is positive, estimators of physical quantities can be obtained by standard importance sampling techniques for classical statistical-mechanical problems, such as the MMC method [22]. If the integrand can become negative severe fundamental difficulties, commonly referred to as "minus sign" problems, may reduce the usefulness of such importance sampling methods considerably. In the next section I discuss this important aspect in more detail.

The VQMC method is certainly the most transparent application of importance sampling concepts to quantum problems. The starting point for any VQMC calculation is a suitable trial wave function which, in general, depends on a set of variational parameters. Many of the recent VQMC calculations have been performed for the 2D S=1/2 Heisenberg antiferromagnet, using different trial wave functions [23-36]. The equivalence between the Heisenberg model and the hard-core boson problem suggest that a Jastrow type of trial state may be appropriate. Indeed, calculations show that it leads to the best overall VQMC results. To get insight into the nature of the ground state, one typically computes spin correlation functions and looks for (off-diagonal) long range order (OD)LRO by calculating the staggered magnetization. The results, a summary of which can be found in [1], reveal that the VQMC suffers from a severe drawback: A trial wave function can have a fairly low energy but nonetheless the correlation functions may differ considerably from those obtained from the exact ground state.

The GFMC method for lattice problems is yet at the very beginning. Up to now it is only applicable to models like the Heisenberg model or the related hard-core boson model [37-39], which have a nodeless ground state wave function. The heart of the GFMC scheme is the well-known power method [40]. From an almost arbitrary state of the system, the ground-state component is filtered out by repeated application of the matrix $G = 1-\tau(H-\omega)$ where H is the hamiltonian and ω is a good guess for the ground state energy. The notion of Green Function stems from the fact that G can be viewed as the series expansion of the imaginary time evolution operator $\exp(-\tau[H-\omega])$ or likewise of the propagator $1/(1+\tau[H-\omega])$ for small "time steps" τ. The iteration scheme converges towards the ground state if the imaginary time step obeys $\tau < 2/(E_{max}-\omega)$ where E_{max} is the spectral radius of H. For many-body problems the spectral radius width generally increases proportionally to N. This implies an increasing number of iterations with increasing system size.

A further and vital element of the GFMC scheme traces back to von Neumann and Ulam [41-43] who proposed the idea to sample the inverse of a matrix by random walks on the index-space of the matrix. One constructs a random walk (Markov chain) on the space of configurations, using the matrix elements of the (approximation to) the Green function to define transition probabilities. In practice it is more economical and also more instructive to follow a whole set of walkers in parallel. Hetherington [44] has nicely illustrated the ideas and shortcomings of the GFMC scheme in terms of (2x2) matrices. He showed the variance of the ground state energy increases exponentially with the number of iterations and decreases only by the usual $1/\sqrt{M}$ with a large number of samples. The variance can be reduced by introducing a guiding function, essentially a trial wave function, thereby making the effective Green function "look more like" a stochastic matrix. Additional problems with this approach are that

1) data are strongly correlated and very careful evaluation of the statistical error is required, otherwise the obtained error bars are much too small,

2) estimates of quantities other than the energy can be inaccurate as it depends on a trial wave function,

3) the method as it stands is only applicable to systems with a real and nodeless ground state wave

function. It is therefore not yet useful for fermionic problems.
Up to now the GFMC method for lattice problems has exclusively been applied to quantum spin problems [37-39,45-47]. Finally it should be mentioned that there is a finite temperature version of this method as well, namely the Handscomb algorithm [48]. This method is particularly geared for the Heisenberg model in that it exploits the spin-1/2 algebra. It has no finite time-step errors. The method has been generalized to the antiferromagnetic Heisenberg model [49-51].

The FTQMC method can be used to study a wide variety of quantum systems. For a review of earlier applications to lattice problems see [52,53]. Recent applications to systems of interacting fermions proceed by eliminating from the partition function, the fermionic degrees of freedom by introducing auxiliary (bosonic) fields. For fermions in continuum space, this leads to the Siegert representation of the grand-canonical partition function [54]. The key elements of deriving this expression are the Feynman path-integral representation for the partition function and the identities for Gaussian integrals to "uncomplete" the square, i.e. to perform the Hubbard Stratonovich (HS) transformation. As the effective fermion action is now a quadratic form of the fermion operators, the trace over the fermions can be carried out analytically. As the auxiliary fields enter Siegert's representation as a consequence of the use a mathematical identity these fields have no proper physical interpretation. Siegert's representation is, at least in principle, amenable to numerical treatment as the integration of the fields can be performed by simulation (e.g. Monte Carlo) methods. The manipulations that transformed the continuum fermion problem into a problem in terms of real numbers can be carried over to lattice fermions without much effort. Instead of starting from the Feynman path integral, one has to invoke the Trotter-Suzuki formula to rewrite the partition function such that the HS transformation can be applied. For some models, notably the Hubbard model, other types of fields may be used as well. In particular, Hirsch [55-57] has introduced a discrete HS transformation in terms of Ising spins. The resulting Ising action has much less phase space than the continuous Gaussian action and is more convenient to sample. A comparative study of the discrete and continuous Hubbard-Stratonovich (HS) transformation has been performed in ref. [58], the conclusion being that the discrete version is superior.

By eliminating the fermionic degrees of freedom in favor of Gaussian or Ising fields, the partition function has been brought into a form suitable for numerical calculations, i.e. it has been expressed entirely in terms of real numbers. The computation time of such algorithms increases with the cube of the system size L and linearly with the number of time-slices m. Moreover, the HS transformation has replaced the many-body Hamiltonian by a one particle Hamiltonian with stochastical fields. The dimension of the involved matrices is hereby drastically reduced from $\binom{L}{N} \times \binom{L}{N}$ (N being the number of spin up and down electrons) to merely $L \times L$. The number of auxiliary fields (proportional to mL) is large and statistical methods have to be invoked to obtain estimates of the relevant quantities. The importance sampling idea is well suited for this task. Unfortunately, a straightforward application of Monte Carlo or Molecular Dynamics methods leads to severe and partly fundamental problems stemming from the quantum nature of the problem. A detailed discussion of these difficulties is relegated to the next section.

The key idea of the (PQMC) method is similar to that of the GFMC algorithm, i.e to filter out the ground state component from a proper trial function by applying an appropriate functional of the Hamiltonian. The numerical realization of this idea, however, is completely different. The PQMC technique employs $\exp(-\beta H)$ as a filter and samples the matrix elements of this operator whereas in the GFMC scheme it is the wave function which is being sampled. To fix the notation we denote the eigenvalues and corresponding eigenvectors of H by $E_0 < E_1 \leq E_2 < \ldots$ and $|\phi_0\rangle$, $|\phi_1\rangle, \ldots$ respectively. Taking an arbitrary state $|\psi\rangle$ it follows from $\lim_{\beta\to\infty} e^{-\beta H}|\psi\rangle/\sqrt{\langle\psi|e^{-\beta H}|\psi\rangle} = |\phi_0\rangle\langle\phi_0|\psi\rangle/|\langle\phi_0|\psi\rangle|$ that projection using $\exp(-\beta H)$ will yield the ground state provided that i) the initial state $|\psi\rangle$ is not orthogonal to $|\phi_0\rangle$ and ii) we let $\beta \to \infty$. Thereby we have tactically

assumed that the ground state is non-degenerate (i.e. $E_0 < E_1$). If the ground-state is nearly degenerate, the convergence of $\exp(-\beta H)|\psi\rangle$ to the true ground-state as a function of β will be slow [59], which is likewise true for the FTQMC scheme. The PQMC scheme can be used to obtain the lowest energy for a given symmetry and allows therefore the determination of certain excitation energies as well [59]. This idea has actually been exploited to compute the low-lying excitation spectrum of the 1D Heisenberg model [60].

To put this projector scheme into practice, a method for computing $\exp(-\beta H)|\psi\rangle$ or more precisely, matrix elements $\langle\phi|\exp(-\beta H)|\psi\rangle$ has to be devised [61,62]. As in the FTQMC approach the basic ingredients of such an algorithm are the Trotter-Suzuki formula and the elimination of interaction terms in favor of auxiliary fields. These ideas have been applied to the Hubbard model and generalizations of it [63-67]. As in the FTQMC approach one has to resort to Monte Carlo like methods to sum over all configurations of auxiliary fields, thereby encountering the same fundamental difficulties. Nevertheless it turns out that this method yields reliable results for a restricted range of model parameters.

None of the quantum simulation methods has provided evidence that the ground state of the 2D single-band Hubbard model or the three-band (Emery) model is superconducting. To examine the interplay of the strong on-site repulsion and a convential pairing mechanism, interaction of the electrons with local (anharmonic) modes has been included. Not unexpectedly, off-diagonal longe range order was found to occur for reasonable (from the point of view of the high-T_c materials) values of the model parameters, e.g. with strong on-site repulsion. Although predictable from handwaving theoretical arguments, the fact that simulations can distinguish between a normal and a superconducting state is a non-trivial result. For the models studied this is mainly due to the short (compared to the size of the lattice) coherence length of the pairs that form the condensate.

Finally some general comments on the Quantum Monte Carlo approach to lattice fermion systems are in order. First of all one should keep in mind that in general none of the algorithms is exact in the sense that even in principle it is not obvious that an infinitly long simulation run will yield the correct answer. The fundamental reason is that the probability distribution used to generate the samples is, with a few exceptions, only up to a sign equal to the integrand that appears in the expression for the partition or projector function. Secondly, even if one has succeeded in obtaining reliable estimates for some physical quantities the computational efforts have been such that one is limited to rather small lattices. As shown in ref.[68] pronounced size effects are present, making even a qualitative interpretation of simulation data very difficult.

Fundamental Problem

All currently used QMC schemes for simulating fermions (with the exception of some variational methods) face the problem of having to compute the action of $\exp(-\beta H)$ on an arbitrary wavefunction $|\psi>$, representing a state of the many-body system. Unless one is in the exceptional situation that it is possible to solve the eigenvalue problem for the model Hamiltonian H, there does not yet exists a direct algorithm for calculating the answer. In addition the number of basis states of the many-particle Hilbert space usually is so large that the amount of storage required to represent a state of the system exhausts the capacity of present-day supercomputers. Hence a practical QMC method has to make use of matrix elements only, not of an explicit representation in terms of all the basis states.

An important step in the construction of such a scheme is to reformulate the matrix-valued problem as a number-valued problem, i.e. to remove the limitations due to storage requirements at the cost of CPU time. The standard procedure to accomplish this it to invoke the Trotter-Suzuki formula or, more generally to approximate $\exp(-\beta H)$ by a product formula. Taking matrix

elements, a necessary condition for the product to be positive is that each factor appearing in the product is positive. The necessary and sufficient condition for $\langle\phi|e^{-\beta H}|\Phi\rangle$ to be positive for all $\beta > 0$ is $\langle\phi|H|\Phi\rangle \leq 0$ for all $\phi \neq \Phi$ or, in other words, all nondiagonal matrix elements of H have to be negative [69]. Although this theorem predicts when a particular factor may become negative, it may still happen that the total number of negative factors (for a specific set of ψ_i's) is even such that the contribution is positive. It seems difficult to specify the necessary conditions for having negative contributions but experience learns that it is wise to adopt the point of view that if one of the factors can become negative (according to the conditions of the above theorem), one should expect to encounter negative contributions.

At this point, it is worthwhile to ask the question why negative contributions should bother us at all. In fact they only create difficulties because the sum representing the partition or Green function or projector operator involving a (very) large number of terms, can only be performed by importance sampling methods. In these methods the product of matrix elements enters the expression for probability determining the importance of a particular state. Clearly it is impossible to directly use the product of matrix elements to compute this probability if the former can take negative values. To summarize: Positive nondiagonal matrix elements of H lead to negative matrix elements. In most cases this results in negative values of the weight of a particular configuration ψ_i. In such cases the essential feature of importance sampling, namely the variance-reduction, is lost.

Novel Method

In an attempt to avoid running into the fundamental difficulties from which all current Quantum Monte Carlo methods suffer, a new method has recently been proposed [70]. It is based on the following considerations. As the exact ground state of a fermion system of reasonable size is a superposition of many (say $> 10^6$) basis states, one can consider the model as being unsolvable if all these basis states are needed to obtain a good approximation to the ground state. As in all previous work in this field, one makes the crucial assumption that an accurate representation of the ground state can be constructed by carefully selecting a limited set of basis states which are "important" [71]. For example, in QMC work one typically samples of the order of 10^5 states, most of which are not linearly independent.

Instead of Markov matrices the new method employs unitary (orthogonal in practice) matrices to perform the walk in Hilbert space. From theoretical viewpoint it is yet another procedure to separate the ground state from the rest of the spectrum, just as for instance the (inverse) power method or the Lanczos scheme. There is considerable similarity of between this scheme and Jacobi method for diagonalizing a real symmetric matrix. The main difference is that one concentrates on the smallest eigenvalue (one could as well concentrate on the largest eigenvalue but from physical point of view this is less interesting). This has important practical implications as it allows one to handle very large matrices without having to store them. What is required is that there exists an economical procedure to calculate an arbitrary matrix element of the Hamiltonian. The method has been applied to the 2D single-band Hubbard model [70]. For closed shell systems it reproduces all know exact results for lattices up to 4×4 with considerable less computational effort than required by the PQMC method [70].

Conclusion

Quantum Monte Carlo simulations have undoubtedly added to the present understanding of the behavior of strongly interacting quantum lattice systems. However, most of the QMC results are not numerically exact and the applicability is limited to a fairly small set of models. The fact that

in the last few years there has been a fast growing activity in this field will hopefully increase the usefullnes of the QMC approach to lattice problems.

Acknowledgements

This work is partially supported by the FOM project 90.816 VS-G-C and a supercomputer grant of the NCF (The Netherlands).

References

[1] H. De Raedt, and W. von der Linden, in: The Monte Carlo Method in Condensed Matter Physics, edited by K. Binder (Springer, Berlin, in press)

[2] A.B. Harris, and R.V. Lang, Phys. Rev. 157, 295 (1967)

[3] T.M. Rice, Helv. Phys. Acta 63, 336 (1990)

[4] V.J. Emery, Phys. Rev. Lett. 58, 2794 (1987)

[5] R. Micnas, J. Ranninger, and S. Robaszkiewicz, Rev. Mod. Phys. 62, 113 (1990)

[6] Special edition for the Hubbard model, World Scientific Publishing (1990)

[7] Y. Zhang, and J. Callaway, Phys. Rev. B 39, 9397 (1989)

[8] M. Imada, in: Strongly Correlated Plasma Physics, edited by S. Ichimaru, (North Holland 1990)

[9] K. Saitoh, and S. Takada, J. Phys. Soc. Jpn. 58, 783 (1989)

[10] R.R. dos Santos, Phys. Rev. B 39, 7259 (1989)

[11] M. Imada, N. Nagaosa, and Y. Hatsugai, J. Phys. Soc. 58, 978 (1989)

[12] A. Muramatsu, and W. Hanke, Phys. Rev. B 38, 878 (1988)

[13] G. Dopf, A. Muramatsu, and W. Hanke, Physica C 162, 807 (1989)

[14] J.E. Gubernatis, Phys. Rev. B 36, 394 (1987)

[15] M. Jarrel, and O. Biham, Phys. Rev. Lett. 63, 2504 (1989)

[16] S.R. White, D.J. Scalapino, R.L. Sugar, and N.E. Bickers, Phys. Rev. Lett. 63, 1523 (1989)

[17] R.M. Fye, Phys. Rev B 41, 2490 (1990)

[18] O. Biham, M. Jarrel, and C. Jayaprakash, Phys. Rev. B 41, 2639 (1990)

[19] D.M. Ceperley and M.H. Kalos, In: Monte Carlo Methods in Statistical Physics, edited by K. Binder, (Topics in Current Physics 7, Springer Berlin 1979)

[20] K.E. Schmidt, and M.H. Kalos, In: Applications of the Monte Carlo Method in Statistical Physics, edited by K. Binder, (Topics in Current Physics 36, Springer Berlin 1984)

[21] E.Y. Loh, Jr. and J.E. Gubernatis, In: Electron Phase Transitions, edited by W. Hauke and Y.V. Kopaev, (Elsevier, New York 1990)

[22] K. Binder and D. Stauffer, In: Applications of the Monte Carlo Method in Statistical Physics, edited by K. Binder, (Topics in Current Physics 36, Springer Berlin 1984)

[23] J.L. Hulthén, Ark. Mat. Astr. Fjs. A 26, 1 (1938)

[24] A. Bijl, Physica 7, 860 (1940)

[25] P.W. Kasteleijn, Physica 18, 104 (1952)

[26] W. Marschall, Proc. Roy. Soc. A 232, 64 (1955)

[27] T.A. Kaplan, P.Horsch, and P. Fulde, Phys. Rev. Lett. 49, 889 (1982)

[28] P. Horsch, and T.A. Kaplan,J. Phys. C 16, L1203 (1983)

[29] C. Gros, R. Joint, and T.M. Rice, Phys. Rev. B 36, 381 (1987)

[30] C. Gros, R. Joint, and T.M. Rice, Z. Phys. B 68, 425 (1987)

[31] S.M. Girvin, and A.H. MacDonald, Phys. Rev. Lett. 58, 1252 (1987)

[32] S. Doniach, M. Inui, V. Kalmeyer, and M Gabay, Europhys. Lett. 6, 663 (1988)

[33] P. Horsch, and W. von der Linden, Z. Phys. B 72, 181 (1988)

[34] D.A. Huse and V. Elser, Phys. Rev. Lett. 60, 2531 (1988)

[35] S. Liang, B. Doucot, and P.W. Anderson, Phys. Rev. Lett. 61, 365 (1988)

[36] W. von der Linden, M. Ziegler, and P. Horsch, Phys. Rev. B 40, 7435 (1989)

[37] M. Gross, E. Sanchez-Velasco and E. Siggia, Phys. Rev. B 39, 2484 (1989)

[38] J. Carlson, In: Quantum Simulations, edited by J.D. Doll and J.E. Gubernatis, World Scientific Publishing, Singapore 1990

[39] N. Trivedi and D.M.Ceperley, GFMC study of Quantum Antiferromagnet. (preprint)

[40] J.H. Wilkinson, The Algebraic Eigenvalue Problem (Clarendon, Oxford, 1965)

[41] G.E. Fortsythe and R.A. Leibler, MTAC 4, 127 (1950)

[42] J.M. Hammersley, and D.C. Handscomb, Monte Carlo Methods (Methuen, London 1964)

[43] J.W.Negele and H. Orland, In: Quantum Many-Particle Systems, Frontieres in Physics (Addison-Wesley, 1987)

[44] J.H. Hetherington, Phys. Rev. A 30, 2713 (1984)

[45] M.P. Nightingale and H.W.J. Blöte, Phys. Rev. B 33, 265 (1986)

[46] T.Barnes and G.J. Daniell, Phys. Rev. B 37, 3637 (1988)

[47] T.Barnes and E.S. Swanson, Phys. Rev. B 37, 9405 (1988)

[48] D.C. Handscomb, Proc. Cambridge Phil. Soc. 58, 594 (1962)

[49] D.H.Lee, J.P. Joannoploulos and J.W. Negele, Phys. Rev. B 30, 1599 (1984)

[50] E. Manousakis and R. Salvador, Phys. Rev. Lett. 60, 890 (1988)

[51] E. Manousakis and R. Salvador, Phys. Rev. B 39, 575 (1989)

[52] H. De Raedt and A. Lagendijk, Phys. Rep. 127, 233 (1985)

[53] M. Suzuki, Quantum Monte Carlo Methods, edited by M. Suzuki, Solid State Sciences 74, (Springer, Berlin 1986)

[54] F. Wiegel, Phys. Rep. 16, 59 (1975)

[55] J.E. Hirsch, Phys. Rev. B. 28, 4059 (1983)

[56] J.E. Hirsch, Phys. Rev. Lett. 51, 1900 (1983)

[57] J.E. Hirsch, Phys. Rev. B. 31, 4403 (1985)

[58] G.M. Buendia, Phys. Rev. B 33, 3519 (1986)

[59] H. De Raedt, Comp. Phys. Rep. 7, 1 (1987)

[60] M. Takahashi, Phys. Rev. Lett. 62, 2313 (1989)

[61] S.E. Koonin, G. Sugiyama, and H. Friederich, Proceedings of the International Symposium, Bad Honnef 1982, (Spinger, Heidelberg 1982)

[62] G. Sugiyama and S.E. Koonin, Annals of Physics 168, 1 (1986)

[63] S. Sorella, E. Tosatti, S. Baroni, R. Car, and M. Parrinello, Proceedings of the Adriatico Research Conference "Towards the Theoretical Understanding of the HighT_c Superconductors"/S. Lundqvist, E. Tosatti, M. Tosi, and L. Yu (World Scientific, Singapore 1988)

[64] S. Sorella, S. Baroni, R. Car, and M. Parrinello, Europhys. Lett. 8, 663 (1989)

[65] W. von der Linden, I. Morgenstern, and Phys. Rev. B 41, 4669 (1990)

[66] M. Frick, W. von der Linden, I. Morgenstern, and H. De Raedt, Z. Phys. B - Condensed Matter 81, 327 (1990)

[67] M. Frick, I. Morgenstern, and W. von der Linden, Z. Phys. B - Condensed Matter 82, 339 (1991)

[68] D. Bormann, T. Schneider, and M. Frick, Europhys. Lett. 14, 101 (1991)

[69] R. Bellman, Introduction to Matrix Analysis, (Maple Press, York, PA. 1960)

[70] H. De Raedt and W. von der Linden, "Monte Carlo diagonalization of very large matrices: Application to fermion systems", Int. J. Mod. Phys. C (in press)

[71] J.B. Bronzan and T.E. Vaughan, Phys. Rev. B 39, 11724 (1989)