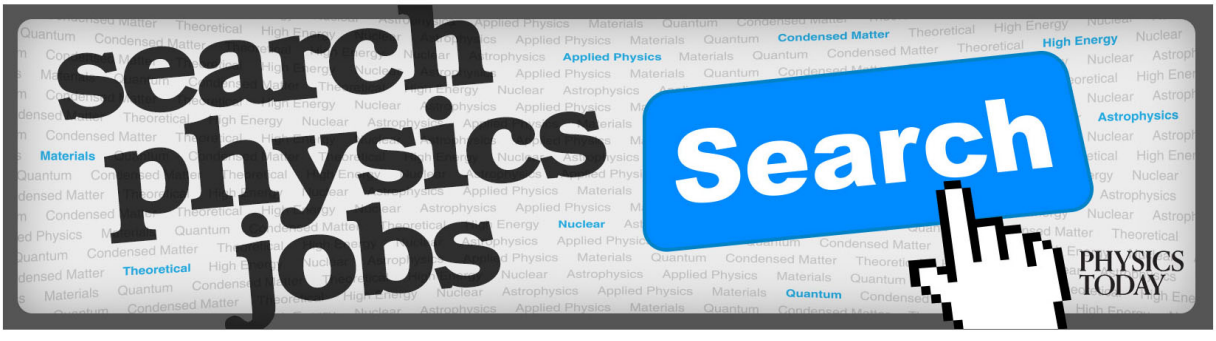
AIP | Journal of Mathematical Physics

Natural Spin-Orbitals and Generalized Overlap Amplitudes

O. Goscinski and P. Lindner

Citation: Journal of Mathematical Physics **11**, 1313 (1970); doi: 10.1063/1.1665261
View online: http://dx.doi.org/10.1063/1.1665261
View Table of Contents: http://scitation.aip.org/content/aip/journal/jmp/11/4?ver=pdfcov
Published by the AIP Publishing



JOURNAL OF MATHEMATICAL PHYSICS VOLUME 11, NUMBER 4 APRIL 1970

Natural Spin-Orbitals and Generalized Overlap Amplitudes*

O. GOSCINSKI AND P. LINDNER
Quantum Chemistry Group for Research in Atomic, Molecular, and Solid-State Theory
Uppsala, Sweden

(Received 31 March 1969)

The generalized overlap amplitudes for "hole" states which appear in the one-particle Green's function are, in general, not linearly independent. We show that canonical orthonormalization of them yields the natural spin-orbitals (eigenfunctions of the first-order reduced density matrix).

INTRODUCTION

The eigenfunctions of the first-order density matrix, introduced by Löwdin as natural spin-orbitals,[1] are an essential tool for treating many-electron systems in stationary states. Their optimal convergence properties have been repeatedly emphasized[1,2] and exploited.[3] They are the most suitable set of 1-particle functions to use in discussing a quantum system, even though their direct determination, without previous knowledge of the wavefunction, is hindered by the N-representability problem.[2]

The first-order density matrix can be considered as an initial value for the 1-particle Green's function of field theory, which is becoming common, even for the treatment of finite electron-systems.[4] A certain set of 1-particle functions,[5] the generalized overlap amplitudes, appears naturally in the spectral weight function of the Green's functions. These overlap amplitudes are characterized by

$$\begin{aligned}\varphi_s(\mathbf{x}) = g_s(\mathbf{x}) &= \langle N, 0|\, \psi^\dagger(\mathbf{x})\, |N-1, s\rangle, \quad \epsilon_s < \mu, \\ &= f_s(\mathbf{x}) = \langle N, 0|\, \psi(\mathbf{x})\, |N+1, s\rangle, \quad \epsilon_s > \mu,\end{aligned} \tag{1}$$

and are associated with the elementary excitations

$$\begin{aligned}\epsilon_s &= E(N, 0) - E(N-1, s), \quad \epsilon_s < \mu, \\ &= E(N+1, s) - E(N, 0), \quad \epsilon_s > \mu,\end{aligned} \tag{2}$$

where $|N, 0\rangle$ denotes the ground state of the N-particle system, $|N+1, s\rangle$ the sth excited state of the $(N+1)$-particle system, $E(N, 0)$ and $E(N+1, s)$ the associated energies, μ the chemical potential, and $\psi(\mathbf{x})$ the field operator in the Heisenberg representation. The spectral weight function, given by

$$A(\mathbf{x}, \mathbf{x}', \epsilon) = \sum_s \varphi_s(\mathbf{x})\varphi_s^*(\mathbf{x}')\delta(\epsilon - \epsilon_s), \tag{3}$$

is important in determining 1-electron properties.

The set $\{g_s(\mathbf{x})\}$, for reasons that we will discuss later, induces the temptation of identifying it with the natural spin-orbitals.[6] The g's have been assumed to be orthonormal,[7] but there is every indication that they are linearly dependent,[8] whereas the natural spin orbitals are orthonormal.[1,2] It has been stated that, except for independent particle models, there is no 1-to-1 correspondence between those many-particle states for which the $\varphi_s(\mathbf{x})$ are different from zero and an orthonormal set.[9]

To make clear the need for a clarification of the relation between the natural orbitals and the generalized overlap amplitudes, we refer to the theory of "capture" and "ionization" processes, where the problem arises naturally and where attempts to establish a connection between the functions we are discussing fail.[10]

In this paper, we establish the connection and derive interrelationships between the $g_s(\mathbf{x})$, the $f_s(\mathbf{x})$, and the natural spin-orbitals, which we will denote by $\chi_i(x)$. In the process, we obtain a derivation of a well-known bound for the occupation numbers of the first-order density matrix. The tool employed is Löwdin's canonical orthonormalization procedure, which is specially devised to cope with linear dependences in a set[11] and which is of importance in the non-orthogonality problem.[12] We briefly review the properties of canonical orthogonalization, density matrices, and field-theoretical Green's functions, then establish the desired connections and discuss the results.

CANONICAL ORTHONORMALIZATION: AN APPLICATION

In order to describe the method, we consider first a basis set, $\boldsymbol{\phi} = \{\phi_k\}$, of n functions which spans a subspace V_p of order p, with $n > p$. The problem is to find a linearly independent basis $\boldsymbol{\varphi}$ for this subspace. The fact that $\boldsymbol{\phi}$ is a linearly dependent set implies that the metric matrix

$$\boldsymbol{\Delta} = \boldsymbol{\phi}^\dagger\boldsymbol{\phi} \tag{4}$$

has p nonvanishing eigenvalues, which are positive since

$$\boldsymbol{\Delta} \geq 0. \tag{5}$$

Let U be the unitary transformation that diagonalizes Δ:

$$U^\dagger \Delta U = d = \begin{pmatrix} \mu & 0 \\ 0 & 0 \end{pmatrix}. \tag{6}$$

The diagonal matrix d has p nonvanishing eigenvalues which can be considered to form a diagonal submatrix μ. From (6), it follows that

$$\Delta U = Ud \tag{7}$$

and

$$\Delta V = V\mu, \quad \Delta A = 0, \tag{8}$$

where V is a partition of U:

$$U = (VA). \tag{9}$$

The matrix U is of order $n \times n$, V is a rectangular submatrix of order $n \times p$, and A of order $n \times q$ with $q = n - p$. It easily follows[12] that

$$V^\dagger V = 1_p, \quad V^\dagger \Delta V = \mu, \quad \Delta = V\mu V^\dagger, \tag{10}$$

where 1_p is a unit matrix of order p. We introduce the set

$$\eta = \phi V \mu^{-\frac{1}{2}}, \tag{11}$$

which has the property

$$\eta^\dagger \eta = \mu^{-\frac{1}{2}} V^\dagger \Delta V \mu^{-\frac{1}{2}} = 1_p. \tag{12}$$

This is the canonical orthonormalization procedure[11,12]; it means that not only are (11) and (12) fulfilled, but also that in V_p we have

$$1 = \eta\eta^\dagger = \sum_{i=1}^{p} |\eta_i\rangle\langle\eta_i|, \tag{13}$$

i.e., the resolution of the identity. We also have

$$\phi = \eta \mu^{\frac{1}{2}} V^\dagger. \tag{14}$$

The transformations (11) and (14) are between two sets of different dimensionality, via rectangular matrices. It can be verified that $\mu^{\frac{1}{2}} V^\dagger$ is the explicit "generalized inverse" of $V\mu^{-\frac{1}{2}}$, which has no ordinary inverse since it is rectangular.[13]

We apply now the preceding results to a seemingly artificial problem in linear spaces which will turn out to be of importance in the next sections. Consider a linear space of dimension p. Assume that there are two sets g and f, each of them of dimension larger than p. We do not assume that either of them is linearly independent. In fact, the only assumptions made are that g contains a linear independent subset of order $r \leq p$ and, what is crucial, that the relation

$$1 = gg^\dagger + ff^\dagger \tag{15}$$

is satisfied. It looks like the resolution of the identity (13), but notice that the analogy is superficial. The g's and the f's form a set with linear dependencies and, of course, with no orthogonality conditions whatsoever imposed on it. Yet, (15) leads to interesting consequences. Canonical orthonormalization of g leads to

$$\chi = gV\mu^{-\frac{1}{2}} \tag{16}$$

and, hence,

$$gg^\dagger = \chi\mu\chi^\dagger. \tag{17}$$

The set χ is orthonormal and of dimension $r \leq p$. Therefore, the resolution of the identity in the space considered is

$$1 = \chi\chi^\dagger + \omega\omega^\dagger, \tag{18}$$

where ω is in the orthogonal complement to χ,

$$\omega^\dagger \chi = \chi^\dagger \omega = 0. \tag{19}$$

If $p = r$, (18) becomes simply $1 = \chi\chi^\dagger$. From (15), (17), and (18) it follows that

$$ff^\dagger = \chi(1_r - \mu)\chi^\dagger + \omega\omega^\dagger. \tag{20}$$

Furthermore, on account of (19),

$$\chi^\dagger f f^\dagger = (1_r - \mu)\chi^\dagger, \tag{21}$$

which means that the relation (15) imposes a bound on the nonvanishing eigenvalues of $g^\dagger g$:

$$\mu_i \leq 1, \quad i = 1, 2, \cdots, r. \tag{22}$$

Trivially,

$$g^\dagger \chi = V\mu^{\frac{1}{2}} \tag{23}$$

and

$$\chi^\dagger g g^\dagger \chi = \mu. \tag{24}$$

Also, from (20), we conclude that, if $\mu = 1_p$, then

$$ff^\dagger = \omega\omega^\dagger \tag{25}$$

and conversely. μ is idempotent in such a case.

FIRST-ORDER DENSITY MATRIX AND NATURAL ORBITALS

The first-order density matrix is defined in terms of the ground-state wavefunction of the N-particle system:

$$\gamma(1 \mid 1') = N \int \Psi(1, 2, \cdots, N) \times \Psi^*(1', 2, \cdots, N)\, dv_2 \cdots dv_N, \tag{26}$$

where 1 denotes the spin-space coordinates of one particle.[1] The kernel $\gamma(1 \mid 1')$ is associated with a nonnegative Hermitian operator γ_{op} of finite trace and, hence, is diagonalizable[1,2,14,15]:

$$\gamma(1 \mid 1') = \sum_i n_i \chi_i(1) \chi_i^*(1'). \tag{27}$$

The χ_i are the natural spin-orbitals[1] and the eigenvalues n_i are the usually called occupation numbers.

Since $\mathrm{Tr}\,\gamma(1 \mid 1') = N$, it follows that

$$\sum_i n_i = N. \tag{28}$$

The Hilbert–Schmidt theory of integral equations[15] implies that the spectrum of n_i consists of a non-increasing sequence of positive numbers which can be finite or infinite. In the latter case, it tends to zero and the χ_i form a complete set in L_2 with optimal convergence properties in the expansion of Ψ.[1,2]

An independent particle model is characterized by $n_1 = n_2 = \cdots = n_N$, in which case γ_{op} is idempotent. Upper and lower bounds for the n_i have been given by several authors. It is well known that[1,2,16]

$$n_i \leq 1. \tag{29}$$

This result has been proven using an expansion of the wavefunction in terms of ordered configurations (Slater determinants)[1] or by using the Schmidt theory[14] of integral equations.[2] Lower bounds have been given,[17] but they involve restricting assumptions on the system.

GREEN'S FUNCTIONS AND GENERALIZED OVERLAP AMPLITUDES

The Green's function[5] is defined by

$$G(1, t; 1', t') = -i\langle T\{\psi(1, t)\psi^\dagger(1', t')\}\rangle. \tag{30}$$

T is the time-ordering operator and the brackets indicate an expectation value with respect to the exact ground state of the interacting system. Atomic units are employed. From (30) and the second quantization form of (26), one gets

$$\gamma(1 \mid 1') = \langle\psi^\dagger(1)\psi(1')\rangle, \tag{31}$$

and it follows that[5,6,8,18]

$$\gamma(1 \mid 1') = -i \lim_{\delta \to 0+} G(1, 0; 1', -\delta). \tag{32}$$

From (30) one can obtain the spectral resolution

$$\begin{aligned} G(1, t; 1', t') &= -i \sum_s f_s(1) f_s^*(1') e^{-i\epsilon_s(t-t')}, \quad t > t', \\ &= i \sum_s g_s(1) g_s^*(1') e^{-i\epsilon_s(t'-t)}, \quad t' > t, \end{aligned} \tag{33}$$

where the f_s, g_s, and ϵ_s are defined in (1) and (2). One gets (33) from (30) by inserting a resolution of the identity between the field operators, where appropriate; this involves states of the $(N + 1)$- or the $(N - 1)$-particle system.

From (32) and (33) it readily follows that[8]

$$\gamma(1 \mid 1') = \sum_s g_s(1) g_s^*(1'). \tag{34}$$

This last equation should be compared with (27). They are both diagonal sums and the temptation of identifying the χ_i with the g_s is great.[6,10] If the g's were orthogonal, their norms would be the occupation numbers. Yet we know that the g's are linearly dependent.[8]

On the other hand, we know that, from the commutation relations of the field operators

$$\psi(1)\psi^\dagger(1') + \psi^\dagger(1')\psi(1) = \delta(1 - 1'), \tag{35}$$

one can obtain a completeness relation for the overlap amplitudes:

$$\sum_s f_s(1) f_s^*(1') + \sum_s g_s(1) g_s^*(1') = \delta(1 - 1'). \tag{36}$$

It is clear from (27) and (34) that we cannot identify the g_s with the χ_i, but there is on the other hand a clue in (36): We have two sets of functions, the f_s and the g_s, neither of which are necessarily linearly independent, but both of which satisfy the completeness relation (36).

NATURAL ORBITALS AND GENERALIZED OVERLAP AMPLITUDES

We notice that the density matrix is the kernel of a completely continuous transformation[19] and that the appearance of a continuum in the expansion (34) does not cause any formal trouble. In fact, this is an ordinary situation: If one formally expresses $\gamma(1 \mid 1')$ in terms of the eigenfunctions of a hydrogen-like operator with a continuum, diagonalization will lead to (27). This is not done in practice, just a conceptual possibility which can be justified.[18] The novelty is not the appearance of the continuum in (34), but the linear dependences.

At this stage we can employ the results which we derived previously with canonical orthonormalization. We assumed before that we dealt with a metric space of order p. Now we deal with an infinite-dimensional space where the completeness relation (36) holds. The set $\mathbf{g} = \{g_1, g_2, \cdots\}$ is, of course, infinite and not discrete, but since

$$\mathrm{Tr}\,\gamma(1 \mid 1') = N, \tag{37}$$

from (34) we conclude that we can form the metric matrix associated to $\mathbf{g}$, and that it has a finite trace, equal to N.

Canonical orthonormalization of the g_s leads to an orthonormal set, and with the preceding assumptions we see that (36) is an extension of (15) and that (17) expresses the interrelationship between (34) and (27). The natural orbitals are thus the canonically orthonormalized overlap amplitudes g_s. The eigenvalues

of the metric matrix associated with the g_s are the occupation numbers of the first-order density matrix.

There are a number of consequences of this connection. From (24) it follows that

$$\sum_s \langle \chi_i \mid g_s \rangle \langle g_s \mid \chi_j \rangle = n_i \delta_{ij}. \tag{38}$$

From (21) we have

$$\sum_s \langle \chi_i \mid f_s \rangle \langle f_s \mid \chi_j \rangle = (1 - n_i)\delta_{ij}. \tag{39}$$

It should be noted that (22) implies (29) and that this derivation of a bound for the occupation numbers required the following prerequisites:

(i) the anticommutation relation (35) in its form (36);

(ii) the formal definition of the Green's function (30) and its connection with the density matrix (32);

(iii) canonical orthonormalization of the set.

The independent-particle model is fully characterized by (25). If the density matrix is idempotent, then $\mathbf{g}^\dagger \mathbf{f} = \mathbf{0}$, i.e., the f's are orthogonal to the g's. Furthermore, the f's are associated with the zero eigenvalue of the density operator and thus represent "empty" orbitals; the set $\{g_s\}$ spans the N-dimensional subspace of the Hilbert space associated with the "occupied" orbitals in an independent-particle model.

We can gain further insight into the problem by examining in more detail the elements of the metric matrix $\mathbf{\Delta} = \mathbf{g}^\dagger \mathbf{g}$:

$$\Delta_{st} = \langle g_s \mid g_t \rangle. \tag{40}$$

Using the definition (1) and a first-quantization representation, we obtain

$$\begin{aligned}\Delta_{st} &= N \int \Psi_t^{N-1*}(2, \cdots, N) \Psi_0^N(1, \cdots, N) \\ &\quad \times \Psi_0^N(1, 2', \cdots, N') \Psi_s^{N-1}(2', \cdots, N')\, dv\, dv' \\ &= \int \Psi_t^{N-1*}(2, \cdots, N) \Gamma_{N,0}^{(N-1)}(2, \cdots, N \mid 2', \cdots, N') \\ &\quad \times \Psi_s(2', \cdots, N') \frac{dv\, dv'}{dv_1\, dv_{1'}}. \end{aligned} \tag{41}$$

Here Ψ_s^{N-1} is the wavefunction of the sth excited state of the $(N-1)$-particle system and $\Gamma_{N,0}^{(N-1)}$ the $(N-1)$th-order reduced density matrix of the ground-state wavefunction of the N-particle system. Therefore, the diagonalization of $\mathbf{\Delta}$ is nothing but the diagonalization of $\Gamma_{N,0}^{(N-1)}$ when the latter is expressed in terms of the eigenfunctions of the $(N-1)$-particle Hamiltonian. Equation (41) confirms that the nonvanishing eigenvalues of $\mathbf{\Delta}$ are the occupation numbers of $\gamma(1 \mid 1')$. This follows from the fact that the nonvanishing eigenvalues of $\Gamma_{N,0}^{(N-1)}$ and of $\Gamma_{N,0}^{(1)} \equiv \gamma$ are identical according to the Carlson–Keller theorem.[2,20] Canonical orthogonalization is required since the eigenvalue zero may occur in both $\Gamma_{N,0}^{(N-1)}$ and $\Gamma_{N,0}^{(1)}$ and, what is worse, with different multiplicity in each case.[20]

Except for a few, if any, bound states, the set f has a norm in the δ-function sense, and the procedure which was used to obtain the natural orbitals from the g's cannot be used. This is most easily seen by considering the quantity analogous to (40); i.e., we study the metric of the f's (we examine the diagonal elements only):

$$\begin{aligned}&\langle f_s \mid f_s \rangle \\ &\quad = \int f_s^*(1) f_s(1)\, dv_1 \\ &\quad = \int \Psi_0^{N*}(1, \cdots, N) \Gamma_{N+1,s}^{(N)}(1, \cdots, N \mid 1', \cdots, N') \\ &\qquad \times \Psi_0(1', \cdots, N')\, dv\, dv'. \end{aligned} \tag{42}$$

We see that the diagonal elements of the metric matrix associated with the f's are expectation values, with respect to the ground state of the N-particle system, of the Nth-order reduced density matrices of the sth excited states of the $(N+1)$-particle system. Since we are dealing with scattering states, the Schmidt theory does not apply in this case.

DISCUSSION

We have shown that the natural spin-orbitals[1] which diagonalize the first-order reduced density matrix are related to the generalized overlap amplitudes of Green's function theory[5–10] by the canonical orthonormalization procedure of Löwdin.[11,12]

This relation, which aroused interest in several contexts,[6,7–10] is established and it leads to orthogonality properties like (38) and (39) and other consequences which follow from (15)–(25).

The natural orbitals provide a basis for expanding the Green's function, for $t < t'$, in a natural way. For $t > t'$, we have no such simple property and a discussion of the zero eigenvalue of $\gamma(1 \mid 1')$ should precede any statement on this.

The results obtained in this paper exploit a connection between conceptual tools sometimes used in a mutually exclusive fashion. An immediate application is to the theory of "capture" and "ionization" processes.[10] Applications to atomic and molecular physics are under way. In treating finite systems, the modifications of external fields (e.g., nuclear

framework, center of mass, etc.) upon changes in the number of particles must be properly treated.

ACKNOWLEDGMENT

We are grateful to Professor P.-O. Löwdin for generous support and stimulating interest.

* Sponsored in part by the Swedish National Research Council and in part by the Air Force Office of Scientific Research (OSR) through the European Office of Aerospace Research (OAR), U.S. Air Force, under Grant EOOAR-69-0043.

[1] P.-O. Löwdin, Phys. Rev. **97**, 1474 (1955); in *Advances in Chemical Physics*, I. Prigogine, Ed. (Interscience Publishers, New York, 1959), Vol. 2, p. 207.

[2] For a review, see A. J. Coleman, Rev. Mod. Phys. **35**, 668 (1963). For updated references and discussions, see *Reduced Density Matrices with Applications to Physical and Chemical Systems* (Queen's Papers on Pure and Applied Mathematics, No. 11), A. J. Coleman and R. M. Erdahl, Eds. (Queen's University, Kingston, Ontario, 1968).

[3] P.-O. Löwdin and H. Shull, Phys. Rev. **101**, A30 (1956). (This is the first "natural analysis" of a wavefunction and it has been followed by many others. See Ref. 2.)

[4] For a review, see J. Linderberg, Magy. Fiz. Folyóirat **16**, 5 (1968). See also J. Linderberg and Y. Öhrn, J. Chem. Phys. **49**, 716 (1968), and references therein. See also L. Hedin, Phys. Rev. **139**, A796 (1965).

[5] They can be found in any textbook on the Green's function method, e.g., A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinski, *Quantum Field Theory in Statistical Physics* (Prentice-Hall, Englewood Cliffs, N.J., 1963).

[6] L. Hedin and S. Lundqvist, Uppsala University, Uppsala, Sweden, Quantum Chemistry Group, TIII, 1960 (unpublished).

[7] G. W. Pratt, Rev. Mod. Phys. **35**, 502 (1963).

[8] L. Hedin, University of Uppsala, Uppsala, Sweden, Quantum Chemistry Group, TN 84, 1962 (unpublished).

[9] L. Hedin, A. Johansson, B. I. Lundqvist, S. Lundqvist, and V. Samathiyakanit, Arkiv Fysik **39**, 97 (1967).

[10] T. Berggren, Nucl. Phys. **72**, 337 (1965); C. F. Clement, Phys. Letters **28B**, 395, 398 (1969).

[11] P.-O. Löwdin, Advan. Phys. **5**, 1 (1956). See also P.-O. Löwdin, Ann. Rev. Phys. Chem. **11**, 107 (1960).

[12] P.-O. Löwdin, University of Uppsala, Uppsala, Sweden, Quantum Chemistry Group, TN 213, 1968 (to be published); P.-O. Löwdin, Intern. J. Quantum Chem. **1S**, 811 (1967).

[13] E. H. Moore, *General Analysis* (American Philosophical Society, Philadelphia, 1935), Vol. 1; R. Penrose, Proc. Cambridge Phil. Soc. **51**, 406 (1955).

[14] E. Schmidt, Math. Ann. **63**, 433 (1907).

[15] F. G. Tricomi, *Integral Equations* (Interscience Publishers, New York, 1957).

[16] F. Sasaki, Phys. Rev. **138**, B1338 (1965).

[17] W. Kutzelnigg and V. H. Smith, J. Chem. Phys. **42**, 2791 (1965).

[18] M. H. Stone, *Linear Transformations in Hilbert Space* (American Mathematical Society Colloquium Publications, New York, 1932), Vol. XV, Chap. VII.

[19] F. Riesz and B. Sz.-Nagy, *Functional Analysis* (F. Ungar Publishing Co., New York, 1955), p. 206.

[20] B. C. Carlson and J. M. Keller, Phys. Rev. **121**, 659 (1961).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 11, NUMBER 4 APRIL 1970

Some Simple Observations on Griffiths' Theorems for the Classical Heisenberg Model*

ROBERT H. T. YEH
Department of Physics and Astronomy, State University of New York Buffalo, New York 14214

(Received 6 November 1969)

We show that Griffiths' theorems are valid for any classical ferromagnetic Heisenberg model in the weak interaction limit. They are also valid for certain chain-type and ring-type models, regardless of interaction strength.

Griffiths[1] has shown that, for an Ising ferromagnet in zero field, with arbitrary crystal structure and range of interaction, the spin correlation obeys two theorems. First, it is nonnegative (Griffiths' first theorem). Furthermore, it is a monotonic increasing function of the interactions (Griffiths' second theorem). These theorems are quite useful and have been generalized in various ways.[2] Recently, it was pointed out[3] that Griffiths' second theorem does not hold for the (quantum) ferromagnetic Heisenberg model because of the existence of a counterexample. It is natural to ask, what is the reason for this difference between the Ising model and the Heisenberg model? Is it due to the quantum nature of spin operators which give rise to some uncertainties in the orientation of each spin vector? Or is it due to the 1-dimensional nature of spin vectors of the Ising model which plays an important role in previous proofs of Griffiths' second theorem? We do not have a complete answer to these questions. However, we show that Griffiths' theorems are valid for the classical ferromagnetic Heisenberg model under certain conditions.

Let

$$\beta H = -\left(\sum_{i>j} J_{ij}\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j + \sum_i B\sigma_{iz}\right),$$

where J_{ij} is the interaction parameter and B is the applied magnetic field. Since temperature is kept