New variational method for quasi-one-dimensional spin problems

1994 J. Phys.: Condens. Matter 6 6651

(http://iopscience.iop.org/0953-8984/6/33/012)

J. Phys.: Condens. Matter 6 (1994) 6651–6658. Printed in the UK

New variational method for quasi-one-dimensional spin problems

V Ya Krivnov and A A Ovchinnikov
Institute of Chemical Physics of Russian Academy of Sciences, 117994 Moscow, Russia

Received 13 December 1993

Abstract. A new variational method for determining the ground-state energy of quasi-1D systems is proposed. The method consists of decomposition of a lattice into non-interacting blocks. A trial wavefunction is the product of exact ground-state block functions multiplied by operator correlation factors. The ground-state energy of a spin-$\frac{1}{2}$ and fermionic particle ladder is evaluated. The calculation is very simple and gives energies with an accuracy of about 2% or even less.

1. Introduction

There has been much interest in low-dimensional, strongly correlated electronic systems and quantum spin models in recent years. There is general agreement that these models are the basis of various theories of high-T_c superconductivity [1].

Exact solutions of these models are known for the 1D case only. Even an investigation of the ground state of quasi-1D and 2D models is a rather complicated problem. Many different methods, such as exact diagonalizations of finite clusters [2–6], Monte Carlo simulations [7–10], perturbation theory [11] and the renormalization group approach [3, 12–15], are used to study these systems. The accuracies of these methods are very different. For example, the real-space renormalization or spin-wave theory used to calculate spin systems gives energies, as a rule, with an accuracy of 10%. More exact estimations are obtained by the Monte Carlo method. However, the quantum Monte Carlo simulation suffers from a 'negative-sign problem' and requires a huge computing time. On the other hand, a finite-size study needs the use of an extrapolation procedure which is rather uncertain. Variational wavefunctions (VWFs) are powerful tools for investigating interacting many-body systems, and many types of VWF [16] have been proposed. One of the most well known is the RVB wavefunction [17], which gives the energy to within 5%. More exact variational estimations [18] demand complicated computer calculations.

Therefore the problem of the construction of a rather simple and reliable VWF is very important.

In this paper we propose a new type of VWF which allows us to estimate singlet ground-state energies with an accuracy of 1–2% and even more exactly by means of simple calculations.

This approach is based on the decomposition of the system into blocks (clusters) with a singlet ground state. The VWF is a product of exact cluster wavefunctions multiplied by a product of correlation factors imitating their interactions. This function can be used both for infinite systems and for finite systems.

0953-8984/94/336651+08$19.50

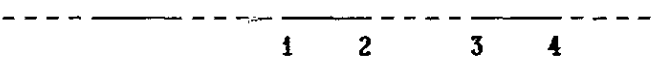

Figure 1. The decomposition of the chain into dimers. The dashed lines denote the correlation factors.

The main object of our consideration is the so-called ladder models which are intermediates between one- and two-dimensional systems. At present, such systems are interesting from experimental and theoretical points of view [4, 19–22]. For example, a spin-$\frac{1}{2}$ ladder may be realized in nature by vanadyl pyrophosphate ($(VO)_2P_2O_7$). It is proposed [4] that it might become a superconductor under hole doping. On the other hand, the fermionic ladder model with a strong interaction between electrons has interesting magnetic properties [22].

2. Variational approach

As a first example we consider the $S = \frac{1}{2}$ Heisenberg linear chain

$$\hat{H} = J \sum_i S_i \cdot S_j. \tag{1}$$

Let us divide it into dimers as in figure 1. The ground state of each dimer is, of course, a singlet with an energy $-\frac{3}{4}J$. We choose the ground-state VWF in the form

$$\Psi = \prod_n T_{2n+1,2n} \Psi_0 \tag{2}$$

where

$$\Psi_0 = \prod_i \varphi(i)$$

and $\varphi(i)$ is the ground-state wavefunction of the ith dimer:

$$\varphi(i) = \frac{1}{\sqrt{2}}(|\alpha\beta) - |\beta\alpha\rangle).$$

The correlation factor $T_{2n-1,2n}$ is an operator which is taken as

$$T_{2n+1,2n} = 1 + \alpha S_{2n+1} \cdot S_{2n} \tag{3}$$

where α is a variational parameter. All factors in equation (2) commute with each other.

The ground-state energy E is

$$E = \langle \Psi H \Psi \rangle / \langle \Psi \Psi \rangle.$$

First we calculate an overlap $N = \langle \Psi \Psi \rangle$. For its calculation we use the obvious equations

$$\langle S_n \rangle_0 = 0 \qquad \langle S_{2n-1} \cdot S_{2n+1} \rangle_0 = -\tfrac{3}{4} \tag{4}$$

where the expectation values were evaluated with respect to Ψ_0. Using equation (4) the overlap N can be obtained trivially (similar to the calculation of a partition function of the 1D Ising model) and N becomes

$$N = \lambda_1^L + 3\lambda_2^L \tag{5}$$

where

$$\lambda_1(\alpha) = (1 + \tfrac{3}{16}\alpha^2) \qquad \lambda_2(\alpha) = -\tfrac{1}{2}\alpha(1 - \tfrac{1}{4}\alpha)$$

and L is the number of dimers. Equation (5) holds for a cyclic chain and for a chain with free ends if the second term is absent. As $|\lambda_2/\lambda_1| < 1$ for all values of α, so for $L \to \infty$,

$$N = \lambda_1^L.$$

The calculation of E is reduced to the calculation of the expectation values $\langle S_{2n-1} \cdot S_{2n}\rangle$ and $\langle S_{2n-1} \cdot S_{2n+1}\rangle$. To find them it is convenient to use the relation

$$(1 + \alpha S_i \cdot S_j)S_i \cdot S_k(1 + \alpha S_i \cdot S_j) = f_1(\alpha)S_i \cdot S_k + f_2(\alpha)S_j \cdot S_k \qquad (6)$$

where

$$f_1(\alpha) = 1 - \tfrac{1}{16}\alpha^2 \qquad f_2(\alpha) = \lambda_2(-\alpha).$$

Using equations (4) and (6) we obtain

$$\langle S_{2n-1} \cdot S_{2n}\rangle = -\tfrac{3}{4}\lambda_1^{L-2} f_1^2(\alpha) \qquad \langle S_{2n} \cdot S_{2n+1}\rangle = -\tfrac{3}{4}\lambda_1^{L-1}\lambda_2(\alpha).$$

Then

$$E = -\tfrac{3}{4}L[(f_1(\alpha)/\lambda_1(\alpha))^2 + \lambda_2(\alpha)/\lambda_1(\alpha)]. \qquad (7)$$

The minimization of E with respect to α is reduced to a quadratic equation and $\alpha_{\min} = (8 - 4\sqrt{13})/9 = -0.7136$. The energy $\varepsilon = E/2L$ per site is

$$\varepsilon = -0.4368J. \qquad (8)$$

This differs by 1.4% from the exact result [23] $\varepsilon = -0.4431J$. In view of the extreme simplicity of calculations the result obtained is in very good agreement with the exact value.

At first sight it seems that it is possible to improve the result by taking four-site clusters (we must divide the chain into clusters with an even number of sites to obtain the singlet ground state). In this case the trial wavefunction has the form

$$\Psi = \prod\prod T_{4n,4n+1}\Psi_0$$

where Ψ_0 is the product of exact ground-state wavefunctions of separate clusters. The calculations lead to the result

$$\varepsilon = -0.4363J.$$

The result obtained is not better than (8). Thus, an increase in the cluster size does not necessarily improve the accuracy, at least for the chain.

Now we consider spin ladder model (two coupled spin chains). The ladder Hamiltonian is

$$\hat{H} = J\sum S_i \cdot S_j + J_\perp \sum S_i \cdot S_j \qquad (9)$$

where S_i is the spin-$\frac{1}{2}$ operator at site i and the first and the second terms describe spin interactions along and across the chains.

We consider some versions of the trial wavefunction of the type (2). The first corresponds to decomposition of the ladder into vertical dimers and the product of the

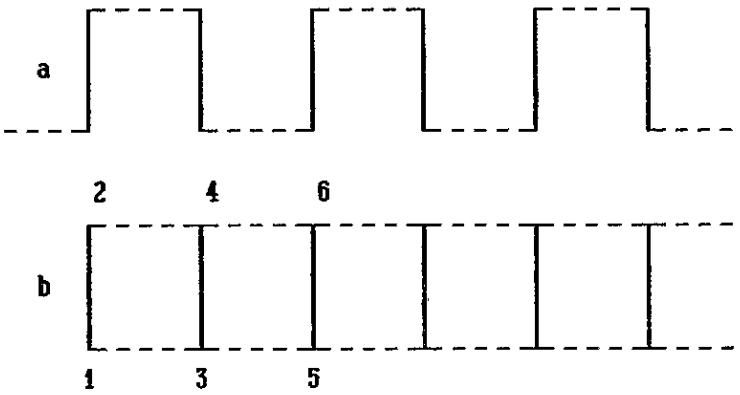

Figure 2. The decomposition of the ladder into dimers. The dashed lines denote the correlation factors. (*a*) and (*b*) correspond to two versions of the VWF.

correlation factors is chosen in accordance with figure 2(*a*), where the dashed lines denote the factors T_{ij}.

The calculation of the overlap N and the expectation values $\langle S_i S_j \rangle$ can be made by analogy with the 1D case. The ground-state energy per site for the isotropic case $J = J_\perp$ is $\varepsilon = -0.5561J$. Even this simplest version of Ψ gives an energy slightly better than short-range RVB approximation ($\varepsilon_{\mathrm{RVB}} = -0.5560J$ [3, 24]). This result can be improved if we choose the VWF in the form shown in figure 2(*b*), i.e.

$$\Psi = T_{13}T_{24}T_{35}T_{46}\ldots\Psi_0. \tag{10}$$

However, in this case the calculation of E differs from previous results and we dwell upon this subject in some detail.

We start with the calculation of the overlap N. We consider the ladder of size L and represent the trial wavefunction in a form

$$\Psi_L = T_{13}T_{24}\Psi_0(1)\Psi_{L-1}$$

where $\Psi_0(1)$ and Ψ_{L-1} are the wavefunctions of the first dimer (exact) and the rest of the ladder. It is easy to show that

$$N_L = \langle \Psi_L \Psi_L \rangle = \lambda_1^2(\alpha) N_{L-1} - 4\lambda_2^2(\alpha)\langle \boldsymbol{S}_3 \cdot \boldsymbol{S}_4 \rangle_{L-1} \tag{11}$$

where the expectation value $\langle \ldots \rangle_{L-1}$ is evaluated with the wavefunction Ψ_{L-1}. It follows from equation (11) that

$$x_L = N_L/N_{L-1} = \lambda_1^2(\alpha) - 4\lambda_2^2(\alpha) y_{L-1} \tag{12}$$

and $y_L = \langle \boldsymbol{S}_1 \cdot \boldsymbol{S}_2 \rangle_L (N_L)^{-1}$ satisfies

$$y_L = \frac{-\frac{3}{4} f_1^2(\alpha) + f_2^2(\alpha) y_{L-1}}{\lambda_1^2(\alpha) - 4\lambda_2^2(\alpha) y_{L-1}}. \tag{13}$$

Equations (12) and (13) allow us to find x_L and y_L by a recursive method beginning with x_1 and y_1. In particular, it turns out that for $L = 2$ (a square) these equations lead to the exact value $\varepsilon = -\frac{1}{2}J$ ($J = J_\perp$).

Equations (15) and (16) have a fixed point at $L \to \infty$ when $x_L \to x$ and $y_L \to y$:

$$y = \frac{\lambda_1^2(\alpha) - f_2^2(\alpha) - \{[\lambda_1^2(\alpha) - f_2^2(\alpha)]^2 + 12\lambda_2^2(\alpha) f_1^2(\alpha)\}^{1/2}}{8\lambda_2^2(\alpha)}$$
$$x = \lambda_1^2(\alpha) - 4\lambda_2^2(\alpha) y. \tag{14}$$

The ground-state energy at $L \to \infty$ is defined by the expectation values $\langle S_{2n-1} \cdot S_{2n+1}\rangle_L$ and $\langle S_{2n-1} \cdot S_{2n}\rangle_L$ when $n \to \infty$. This average satisfies recurrence equations as well. For example, for the first of them we have

$$p_L(n) = a_L p_{L-1}(n) + b_L g_{L-1}(n) \qquad g_L(n) = c_L p_{L-1}(n) + d_L g_{L-1}(n) \tag{15}$$

where

$$p_L(n) = \langle S_{2n-1} \cdot S_{2n+1}\rangle_L / N_L \qquad g_L(n) = \langle (S_1 \cdot S_2)(S_{2n-1} \cdot S_{2n+1})\rangle_L / N_L$$

$$a_L = \lambda_1^2(\alpha)/x_L \qquad b_L = -4\lambda_2^2(\alpha)/x_L \qquad c_L = -3f_1^2(\alpha)/4x_L \qquad d_L = f_2^2(\alpha)/x_L.$$

When $L \to \infty$, $a_L \to a$, $p_L(n) \to p(n)$, $p_{L-1}(n) \to p(n-1)$, etc, equations (15) reduce to

$$p(n) = ap(n-1) + bg(n-1) \qquad g(n) = cp(n-1) + dg(n-1) \tag{16}$$

with the initial conditions

$$p(2) = \langle S_1 \cdot S_3\rangle_L / N_L \qquad g(2) = \langle (S_1 \cdot S_2)(S_3 \cdot S_5)\rangle_L / N_L.$$

The equations for limiting values $u(n)$ and $v(n)$, where

$$u(n) = \langle S_{2n-1} \cdot S_{2n}\rangle_L / N_L \qquad v(n) = \langle (S_1 \cdot S_2)(S_{2n-1} \cdot S_{2n})\rangle_L / N_L \qquad L \to \infty$$

have the same form as equations (16). The solutions of equations (16) are

$$p(n) = A_1\mu_1^n + A_2\mu_2^n \qquad g(n) = A_3\mu_1^n + A_4\mu_2^n \tag{17}$$

where $\mu_{1,2}$ satisfy the equation

$$\mu^2 - \mu(a+d) + ad - bc = 0.$$

Taking into account equation (14) it is easy to show that $\mu_1 = 1$ while

$$\mu_2 = a(\alpha) + d(\alpha) - 1 < 1.$$

This means that $p(n)$ ($u(n)$) and $g(n)$ ($v(n)$) tend to constants when $n \to \infty$ as they should do. The second terms in equation (17) are end effects. (For the cyclic ladder, all $p(n) = A_1$.) Thus, $p(n) \to A_1$ and A_1 is

$$A_1 = \frac{p(2)[d(\alpha) - 1] - g(2)b(\alpha)}{a(\alpha) + d(\alpha) - 2}.$$

The ground-state energy ε per site is

$$\varepsilon = \frac{[p(2) + u(2)][d(\alpha) - 1] - [g(2) + v(2)]b(\alpha)}{2[a(\alpha) + d(\alpha) - 2]}. \tag{18}$$

The initial values $p(2)$, $g(2)$, $u(2)$ and $v(2)$ can be found from equations which are analogous to equations (12)–(14). For example,

$$u(2) = [f_1^2(\alpha)y - \tfrac{3}{4}f_2^2(\alpha)](x)^{-1}.$$

Minimizing equation (18) with respect to α, we arrive at

$$\varepsilon = -0.5740J \qquad \alpha_{\min} = -0.55 \tag{19}$$

for $J = J_\perp$. This value differs by 0.7% from the value $\varepsilon = -0.578J$ obtained in [3, 6] by the extrapolation of numerical calculations of finite clusters.

One more version of VWF corresponds to decomposition of the ladders into squares (figure 3):

$$\Psi = \prod T_{ij}\Psi_0 \tag{20}$$

where Ψ_0 is the product of the exact singlet ground-state wavefunctions of separate squares. We note that all the factors T_{ij} commute with each other, in contrast with the preceding version. For $J_\perp = 0$ the wavefunction (20) coincides with a product of two 1D wavefunctions (2). The ground-state energy can be found by the recursive procedure by analogy with the preceding. However, it is easier to act somewhat differently. Let us consider a cyclic (in a long direction) ladder. Then we need three types of expectation value, making the contributions $\langle S_3 \cdot S_4\rangle$, $\langle S_1 \cdot S_3\rangle$ and $\langle S_3 \cdot S_5\rangle$ to the ground-state energy. Using the fact that all factors T_{ij} commute with each other, it is possible to represent, for example, $\langle S_3 \cdot S_4\rangle$ as

$$\langle \Psi S_3 \cdot S_4 \Psi\rangle = \langle \Psi_{L'}, T_{35}T_{46}S_3 \cdot S_4 T_{46}T_{35}\Psi_{L'}\rangle \tag{21}$$

where $\Psi_{L'}$ ($L' = L - 1$) is the wavefunction of the ladder with free ends. We note that the correlation factors in equation (10) do not commute with each other and their order in equation (10) cannot change.

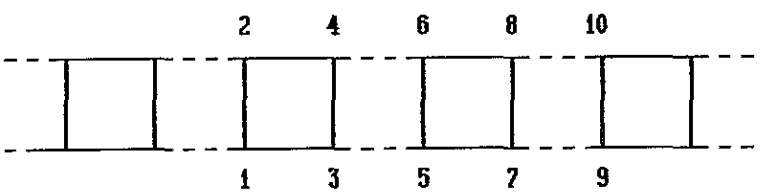

Figure 3. The decomposition of the ladder into squares.

Using equation (6) it is possible to represent equation (21) in the form

$$\langle \Psi S_3 \cdot S_4 \Psi\rangle = f_1^2(\alpha)\langle S_3 \cdot S_4\rangle_{L'} + f_2^2(\alpha)\langle S_5 \cdot S_6\rangle_{L'} + f_1(\alpha)f_2(\alpha)[\langle S_4 \cdot S_5\rangle_{L'} + \langle S_3 \cdot S_6\rangle_{L'}]. \tag{22}$$

The last term in equation (22) vanishes when $L \to \infty$ while $\langle S_3 \cdot S_4\rangle_{L'}$ and $\langle S_5 \cdot S_6\rangle_{L'}$ are expectation values of scalar products corresponding to the first and the last squares of the ladder with free ends. It is evident that $\langle S_3 \cdot S_4\rangle_{L'} = \langle S_5 \cdot S_6\rangle_{L'}$. These expectation values can be found in a manner analogous to the way that it was done in the derivation of equation (14). The same method can be used to calculate the expectation values $\langle S_1 \cdot S_3\rangle$ and $\langle S_3 \cdot S_5\rangle$.

As a result we obtain for the energy per site in the isotropic case

$$\varepsilon = -0.5741J \qquad \alpha_{\min} = -0.52. \tag{23}$$

This value almost coincides with ε from (19).

Table 1. Variational and extrapolated [6] results for the ground energy per site of spin ladder.

$J_\perp/J$	$\alpha_{\min}$	ε/J	$(\varepsilon/J)_{\text{extr}}$	Error (%)
0.0	−0.714	−0.437	−0.443	1.4
0.2	−0.721	−0.443	−0.453	2.2
0.4	−0.733	−0.461	−0.472	2.3
0.6	−0.691	−0.492	−0.500	1.6
0.8	−0.601	−0.530	−0.535	0.9
1.0	−0.520	−0.574	−0.578	0.7
2.0	−0.271	−0.858	−0.859	0.1

We also calculate the ground-state energies for different values of the anisotropy parameter $J_\perp/J$ in the range $0 \leqslant J_\perp/J \leqslant 2$. These data are presented in table 1 together with estimates obtained by extrapolation of finite-size calculations in [6]. It is seen from table 1 that differences between our data and the extrapolated data do not exceed 2.3%.

Up to this point our treatment has pertained to spin systems. However, this approach can be generalized without difficulty to Fermi systems. As an example, we consider a ladder described by the Hubbard Hamiltonian with $U = \infty$:

$$\hat{H} = -t \sum_{\langle ij \rangle} (a_{i\sigma}^+ a_{j\sigma} + a_{j\sigma}^+ a_{i\sigma}) \tag{24}$$

where $\langle ij \rangle$ denotes nearest neighbours and the operators $a_{i\sigma}^+$ are connected with the original Fermi operators $c_{i\sigma}^+$ by the relation

$$a_{i\sigma}^+ = c_{i\sigma}^+ (1 - c_{i,-\sigma}^+ c_{i,-\sigma}).$$

The magnetic properties of this model were studied by us [22] in the framework of the auxiliary-space approach. In particular, it was shown that the ground state is a singlet at $\rho = \frac{1}{2}$ (ρ is the number of electrons per site). Below we shall obtain a variational estimate of the energy of this state.

We decompose the ladder into squares as in figure 3. The VWF is chosen as

$$\Psi = (1 + \alpha T_{35} + \alpha T_{46})(1 + \alpha T_{79} + \alpha T_{8,10}) \ldots \Psi_0 \tag{25}$$

where Ψ_0 is a product of the exact ground-state wavefunctions of squares, containing two electrons (this guarantees that $\rho = \frac{1}{2}$) and

$$T_{ij} = \sum_\sigma (a_{i\sigma}^+ a_{j\sigma} + a_{j\sigma}^+ a_{i\sigma}).$$

Since the correlation factors T_{ij} commute with each other, it is possible to calculate the expectation values $\langle T_{34} \rangle$, $\langle T_{13} \rangle$ and $\langle T_{35} \rangle$, which are contributions to the energy, using formulae of the type (21).

For the (2×4) ladder the calculation gives the energy ε per site as $-0.736t$ compared with the exact result $\varepsilon = -0.748t$ [25]. The error is 1.6%. For $L \to \infty$ we obtained $\varepsilon = -0.771t$. The exact value of ε is unknown. An extrapolation of the results of exact diagonalizations [25, 26] of a ladder with $L = 2, 4, 6$ using an asymptotic form

$$\varepsilon = a + \frac{b}{L} + \frac{c}{L^2}$$

gives $\varepsilon = -0.785t$.

3. Summary

Our considerations have shown that the proposed VWF gives a good accuracy (about 2% or less) of the singlet ground-state energy of 1D and quasi-1D ladder systems. In any case, these estimates are better than obtained by the short-range RVB *ansatz*. It should be stressed that the calculation based on the proposed approach is very simple, especially if the version of the VWF with commuting correlation factors is used. This approach can be easily generalized to more complicated models than defined by equation (1) or (24). For example, it is possible to consider the models with not only nearest-neighbour interactions and/or for other than the $S = \frac{1}{2}$ spin value.

Unfortunately, its application to 2D or 3D systems meets difficulties. For example, expectation values of the type $\langle (S_i \cdot S_j)(S_j \cdot S_k) \dots (S_l \cdot S_i) \rangle$ appear when we calculate the energy and it is necessary to sum the contributions of these averages, beginning and ending at the same cluster. In this connection it is worth noting that the value of $|\alpha_{\min}|$, as follows from table 1, reduces from 0.71 for a chain to 0.52 for a ladder. This confirms a decrease of about $|\alpha_{\min}|$ for systems of higher dimensionality. This indicates the possibility of using perturbation theory in α. This problem needs further investigations.

Acknowledgments

We are grateful to Professor D J Klein and Dr V O Cheranovskii for useful discussions relating to this work. This work was supported by Russian Fund of Fundamental Investigations under grants 93-03-18639 and 93-03-18538.

References

[1] Anderson P W 1987 *Science* **235** 1196
[2] Oitmaa J and Bets D D 1978 *Can. J. Phys.* **56** 897
[3] Zivcovic T P, Sandleback B L, Schmalz T G and Klein D J 1990 *Phys. Rev.* B **41** 2249
[4] Dagotto E, Riera J and Scalapino D 1992 *Phys. Rev.* B **45** 5744
[5] Johnson M O and Subbaswamy K R 1988 *Phys. Rev.* B **37** 9390
[6] Barnes T, Dagotto E, Riera J and Swanson E S 1993 *Phys. Rev.* B **47** 3196
[7] De Raedt H and von der Linden W 1992 *The Monte Carlo Method in Condensed Matter Physics* ed K Binder (Berlin: Springer)
[8] Carlson J 1989 *Phys. Rev.* B **40** 846
[9] Reger J D and Young A P 1988 *Phys. Rev.* B **37** 5978
[10] Barnes T and Swanson E S 1988 *Phys. Rev.* B **37** 9405
[11] Huse D A 1988 *Phys. Rev.* B **37** 2380
[12] Caspers W J 1980 *Phys. Rep.* **63** 224
[13] Mattis D C and Pan C Y 1988 *Phys. Rev. Lett.* **61** 463
[14] Hirsch J E 1980 *Phys. Rev.* B **22** 5259
[15] Hite G E, Metropoulos A, Klein D J, Schmalz T G and Seitz W A 1986 *Theor. Chim. Acta* **69** 393
[16] Vollhardt D 1989 *Interacting Electrons in Reduced Dimension* ed D Baeryswyl and D C Campbell (New York: Plenum)
[17] Anderson P W 1973 *Mater. Res. Bull.* **8** 153
[18] White S R 1992 *Phys. Rev. Lett.* **69** 2863
[19] Johnston D C, Johnson J W, Goshozn D P and Jacobson A J 1987 *Phys. Rev.* B **35** 219
[20] Dagotto E and Moreo A 1988 *Phys. Rev.* B **38** 5087
[21] Hida K 1991 *J. Phys. Soc. Japan* **60** 1347
[22] Krivnov V Ya and Ovchinnikov A A 1992 *Phys. Rev.* B **45** 12996
[23] Hulthen L 1938 *Ark. Mat. Astron. Fys.* A **26** 1
[24] Fan Y and Ma M 1988 *Phys. Rev.* B **37** 1820
[25] Takahashi M 1982 *J. Phys. Soc. Japan* **51** 3475
[26] Cheranovskii V O 1991 unpublished