

## Single-hole state in the half-filled Hubbard model. The coupled-cluster method

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We have investigated the ground state of a single hole in the half-filled Hubbard model on a 2D square lattice using the coupled-cluster method. In the strong-coupling limit we have obtained an analytical expression of the hole energy dispersion  $\epsilon(\mathbf{k})$  with several of its features consistent with earlier studies of the Hubbard model and  $t$ - $J$  model. An appreciable discrepancy on the hole bandwidth is, however, found between the Hubbard model and the  $t$ - $J$  model. We believe that this discrepancy is due to the absence of the three-site hopping term in the  $t$ - $J$  model.

In the past few years the high temperature superconductors have been widely studied, both theoretically and experimentally. It has been suggested [1] that the nearly half-filled, two-dimensional (2D) Hubbard model in the large Coulomb repulsion limit might be relevant to the physics of high temperature superconductors. In the strong coupling limit  $t/U \ll 1$  and using second-order perturbation theory, the nearly half-filled Hubbard model can be further simplified to what is called the  $t$ - $J$  model. This model has now become the focus of theoretical studies. An effort has been made recently to study the properties of the ground state of a single hole by a number of authors both analytically and numerically [2-4]. Some of the properties of the single-hole state are by now well established while others, e.g. the position of the minimum of the hole energy band and the scaling of the bandwidth with  $J$ , are still controversial. It is, therefore, desirable to further investigate the single-hole problem by an independent approach. Furthermore, it is of interest to check whether the  $t$ - $J$  model suffices to represent accurately the single-band Hubbard model in the large Coulomb repulsion limit.

In the present work we have investigated the ground state of a single hole in the half-filled Hubbard model on a 2D square lattice using a reformulation [5] of the coupled-cluster method [6]; this quantum many-body technique has proven useful in a wide variety of fields ranging from quantum chemistry to nuclear physics. The coupled-cluster approach, which overcomes the limitations of dealing with small-size lattices, may provide both an analytical understanding of the nature of the correlations introduced by the hole and a deeper insight in the possibility of hole pairing. More importantly, this new scheme of successive coupled-cluster approximations enables us to dig up the underlying physics in a very systematic manner. In this paper we have obtained an analytical expression of the hole energy dispersion  $\epsilon(\mathbf{k})$  in the strong-coupling limit; this dispersion function reproduces several major features that have been found in earlier studies of the Hubbard model and  $t$ - $J$  model. However, as shown both by our calculations and the exact diagonalization of the Hubbard model on a ten-site lattice, an appreciable discrepancy on the hole bandwidth exists between the Hubbard model and the  $t$ - $J$  model. We believe that this discrepancy is due to the absence of the three-site hopping term in the  $t$ - $J$  model. This, in turn, implies that the  $t$ - $J$  model does not suffice to describe accurately the basic features of the Hubbard model in the large Coulomb repulsion limit.

The basic idea of the coupled-cluster method can be outlined as follows: The ground state of a many-body Hamiltonian  $H$  can be expressed as

$$|\Psi\rangle = \exp(S) |\Phi_0\rangle, \quad (1)$$

with  $|\Phi_0\rangle$  being an appropriate "starting wave function" which is not orthogonal to the exact ground state. The Schrödinger equation

$$H|\Psi\rangle = E_0|\Psi\rangle \quad (2)$$

can then be written as

$$\mathcal{H}|\Phi_0\rangle \equiv \exp(-S)H\exp(S)|\Phi_0\rangle = E_0|\Phi_0\rangle, \quad (3)$$

where

$$\exp(-S)H\exp(S) = H + [H, S] + \frac{1}{2!} [[H, S], S] + \dots \quad (4)$$

Since  $|\Phi_0\rangle$  is normalized, we may write

$$\langle \Phi_0 | \mathcal{H} | \Phi_0 \rangle = \langle \Phi_0 | \exp(-S)H\exp(S) | \Phi_0 \rangle = E_0, \quad (5)$$

and by projecting eq. (3) onto the states  $|\Phi_n\rangle$  which are orthogonal to  $|\Phi_0\rangle$  we obtain

$$\langle \Phi_n | \mathcal{H} | \Phi_0 \rangle = \langle \Phi_n | \exp(-S)H\exp(S) | \Phi_0 \rangle = 0. \quad (6)$$

This orthogonality condition yields a series of nonlinear coupled equations, each of which contains a finite number of terms. The correlation operator  $S$  is determined by solving these equations. Once  $S$  is known, the ground-state energy and wave function can be obtained readily. Hence, the problem of finding the ground-state energy and wave function of the many-body system is reduced to computing the operator  $S$ . Nevertheless, this is a very formidable task, and we have to resort to some approximation scheme to solve the coupled equations. In the following we will apply a successive coupled-cluster approximation scheme to investigate the ground state of a single hole in the half-filled Hubbard model on a 2D square lattice. This approximation was recently proposed by Roger and Hetherington [5] and has been successfully applied to the antiferromagnetic Heisenberg linear chain and the half-filled Hubbard model on a square lattice.

The Hamiltonian of the single-band Hubbard model is given by

$$H = -t \sum_{\langle i,j \rangle, \sigma} C_{i-\sigma}^\dagger C_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}. \quad (7)$$

Anticipating antiferromagnetism in the half-filled case, we have rotated the quantization axis at each site of one sublattice (down) into the direction of the local mean field, as evidenced by the  $-\sigma$  subscript in eq. (7). We choose the single-hole state with momentum  $\mathbf{k}$  to be given by

$$\exp(S)|\mathbf{k}\rangle = \exp(S) \frac{1}{\sqrt{N}} \sum_i \exp(i\mathbf{k}\cdot\mathbf{r}_i) C_{i\uparrow} |\text{Néel}\rangle, \quad (8)$$

where the Néel state is taken to be the state with all spins "up":  $|\text{Néel}\rangle \equiv \prod_{i=1}^N C_{i\uparrow}^\dagger |\text{vacuum}\rangle$  in this new basis. For the first level of the successive coupled-cluster approximation (CCA) scheme, we simply include in  $S$  the operators which move one electron onto a neighbouring site:

$$S = \alpha_1 \sum_{\langle i,j \rangle} C_{i\downarrow}^\dagger C_{j\uparrow}, \quad (9)$$

where the parameter  $\alpha_1$  is to be determined. Using this correlation factor  $S$ , we obtain

$$\exp(-S)H \exp(S)|\mathbf{k}\rangle = \left( E(\mathbf{k}) + F_1 \sum_{\langle i,j \rangle}^{(1)} C_{i_l}^\dagger C_{j_t} + F_2 \sum_{\langle i,j \rangle}^{(1)} C_{i_l}^\dagger C_{j_t} (1 - n_{i_t}) + F_3 \sum_{\langle i,j \rangle}^{(1)} C_{i_l}^\dagger C_{i_t} C_{j_l}^\dagger C_{j_t} \right. \\ \left. + F_4 \sum_{\langle i,j \rangle}^{(1)} \sum_{k \langle j \rangle \neq i}^{(1)} C_{i_l}^\dagger C_{j_t} C_{j_l}^\dagger C_{k_t} + F_5 \sum_{\langle i,j \rangle}^{(4)} C_{i_l}^\dagger C_{j_t} + F_6 \sum_{\langle i,j \rangle}^{(6)} C_{i_l}^\dagger C_{j_t} \right) |\mathbf{k}\rangle, \quad (10)$$

where  $E(\mathbf{k}) = -4Nt\alpha_1 + t\alpha_1\gamma(\mathbf{k})^2$ ,  $F_1 = U\alpha_1 - t + 9\alpha_1^2 t$ ,  $F_2 = U\alpha_1$ ,  $F_3 = -F_4 = U\alpha_1^2$ ,  $F_5 = 3F_6 = 3t\alpha_1^2$ . Here the sums  $\sum_{\langle i,j \rangle}^{(n)}$  are restricted to first, fourth and sixth neighbours in terms of Euclidean distance, with  $n=1, 4, 6$  respectively, and the sum  $\sum_{j \langle i \rangle}^{(1)}$  denotes summation over nearest neighbour sites around site  $i$ . The parameter  $\alpha_1$  is obtained by setting the coefficient of the second term in eq. (10) to zero:

$$\alpha_1 = \frac{\sqrt{1 + 36(t/U)^2} - 1}{18t/U},$$

and the hole energy is given by  $\epsilon(\mathbf{k}) = t\alpha_1\gamma(\mathbf{k})^2$  with

$$\gamma(\mathbf{k}) = \sum_{j \langle i \rangle}^{(1)} \exp[i\mathbf{k} \cdot (\mathbf{r}_j - \mathbf{r}_i)] = \sum_{i \langle 0 \rangle}^{(1)} \exp(i\mathbf{k} \cdot \mathbf{r}_i) = 2[\cos(k_x) + \cos(k_y)].$$

Then in the next level of approximation we also include in  $S$  the terms necessary to cancel the remaining terms of eq. (10):

$$S = \alpha_1 \sum_{\langle i,j \rangle}^{(1)} C_{i_l}^\dagger C_{j_t} + \alpha_2 \sum_{\langle i,j \rangle}^{(1)} C_{i_l}^\dagger C_{j_t} (1 - n_{i_t}) + \alpha_3 \sum_{\langle i,j \rangle}^{(1)} C_{i_l}^\dagger C_{i_t} C_{j_l}^\dagger C_{j_t} + \alpha_4 \sum_{\langle i,j \rangle}^{(1)} \sum_{k \langle j \rangle \neq i}^{(1)} C_{i_l}^\dagger C_{j_t} C_{j_l}^\dagger C_{k_t} \\ + \alpha_5 \sum_{\langle i,j \rangle}^{(4)} C_{i_l}^\dagger C_{j_t} + \alpha_6 \sum_{\langle i,j \rangle}^{(6)} C_{i_l}^\dagger C_{j_t}. \quad (11)$$

Here the first, fifth and sixth terms represent single hops of an electron to the first, fourth and sixth neighbour sites respectively, while the second is the nearest neighbour hole-hopping term. The third term denotes the nearest neighbour spin exchange, and the fourth represents double hops of an electron involving three nearest neighbours (aligned or at the corner of a triangle). After some tedious but straightforward algebra, we find an expression like eq. (10) with different  $E(\mathbf{k})$  and  $F_i$ , plus extra terms which are to be neglected at this level of approximation. By setting the coefficients to zero, a set of six nonlinear coupled-cluster equations of the parameters  $\alpha_i$  are obtained, which has no closed-form solution in general [7]. Thus, we have used the Levenberg-Marquardt algorithm [8] to solve these coupled equations. The hole energy  $\epsilon(\mathbf{k})$  is given by

$$\epsilon(\mathbf{k}) = -4t(\alpha_2 + 2\alpha_5 + \alpha_6) + t\gamma_1(\mathbf{k})[\alpha_1\gamma_1(\mathbf{k}) + \alpha_5\gamma_4(\mathbf{k}) + \alpha_6\gamma_6(\mathbf{k})], \quad (12)$$

where  $\gamma_n(\mathbf{k}) = \sum_{i \langle 0 \rangle}^{(n)} \exp(i\mathbf{k} \cdot \mathbf{r}_i)$ , with the sums  $\sum_{i \langle 0 \rangle}^{(n)}$  denoting summations over first, fourth and sixth neighbour sites around site  $i$ , with  $n=1, 4$  and  $6$  respectively. Here

$$\gamma_1(\mathbf{k}) = 2[\cos(k_x) + \cos(k_y)], \quad \gamma_4(\mathbf{k}) = 4[\cos(2k_x)\cos(k_y) + \cos(k_x)\cos(2k_y)],$$

$$\gamma_6(\mathbf{k}) = 2[\cos(3k_x) + \cos(3k_y)].$$

Note that only the terms involving single hops of an electron to the first, fourth and sixth neighbour sites are explicitly responsible for the dispersion of  $\epsilon(\mathbf{k})$ , and that along the direction  $(\pi, 0)$  to  $(0, \pi)$  in the Brillouin zone all the three  $\gamma_i(\mathbf{k})$  vanish and the dispersion curve is flat.

In the large  $U$  limit, retaining the lowest-order term in  $t/U$ , the CCA equations lead to:  $\alpha_1 = 10t/7U$ ,  $\alpha_2 = \sqrt{2/5}$ ,  $\alpha_3 = -3/14$ ,  $\alpha_4 = -\alpha_1/\sqrt{10}$ , with the other two parameters of order  $(t/U)^3$ , and the hole energy is

$$\epsilon(\mathbf{k}) = -4t\alpha_2 + t\alpha_1\gamma_1(\mathbf{k})^2 = -4\sqrt{2/5}t + 10\gamma_1(\mathbf{k})^2 t^2/7U.$$

It is clear that the hole energy dispersion function has a minimum value of  $-2.5298t$  at the zone boundary, which at this level of approximation is degenerate, and attains its maximum at  $\mathbf{k}=(0, 0)$  and  $(\pi, \pi)$ . Thus, the hole energy bandwidth, defined as the difference between  $\epsilon_{\max}$  and  $\epsilon_{\min}$ , is given by  $W=160t^2/7U=40J/7$ . Also, the effective mass of the hole is much smaller in the direction  $(0, 0)$  to  $(\pi, \pi)$  than in the direction  $(0, \pi)$  to  $(\pi, 0)$ . These results are in agreement with the qualitative statements made in previous studies of the  $t$ - $J$  model [2-4], except that the hole bandwidth  $W$  is much larger in the Hubbard model. To remove the degeneracy along the zone boundary, one needs to include in  $S$  the terms  $S_7=\alpha_7 \sum_{\langle l,j \rangle} \sum_{k \in \mathcal{Z}_2} C_l^\dagger C_{k+l}(1-n_{j+l})$  and  $S_8=\alpha_8 \sum_{\langle l,j \rangle} \sum_{k \in \mathcal{Z}_3} C_l^\dagger C_{k+l}(1-n_{j+l})$ , where the sums  $\sum_{k \in \mathcal{Z}_n}$  denote summation over second and third neighbour sites around site  $j$ , with  $n=2$  and  $3$  respectively. These two terms are among the extra terms generated in the second level of CCA, and should be included in the next level of approximation. It is not difficult to see that the inclusion of these two terms will modify the hole energy dispersion  $\epsilon(\mathbf{k})$  to

$$\epsilon(\mathbf{k}) = -4t(\alpha_2 + 2\alpha_5 + \alpha_6 + 2\alpha_7 + \alpha_8) + t\gamma_1(\mathbf{k})[\alpha_1\gamma_1(\mathbf{k}) + \alpha_5\gamma_4(\mathbf{k}) + \alpha_6\gamma_6(\mathbf{k})] + 4t\alpha_7\gamma_2(\mathbf{k}) + 4t\alpha_8\gamma_3(\mathbf{k}), \quad (13)$$

where

$$\gamma_2(\mathbf{k}) = 4 \cos(k_x) \cos(k_y), \quad \gamma_3(\mathbf{k}) = 2[\cos(2k_x) + \cos(2k_y)].$$

Clearly, the degeneracy along the zone boundary is now lifted, and the bottom of the band occurs at  $(\pi/2, \pi/2)$ . The band is anisotropic near the minimum with the "heavy" mass along the zone boundary and the "light" mass in the direction perpendicular (toward the zone center). The determination of the parameters  $\alpha_i$ , however, requires more lengthy calculations, and the results will be reported later [7]. Nevertheless, we believe that these two new terms will provide small corrections only.

As mentioned above the set of six nonlinear coupled-cluster equations has no closed-form solution, and thus we have to solve these equations numerically to determine the parameters  $\alpha_i$  for different values of  $t/U$ . With these numerical results we are able to calculate the hole energy dispersion function  $\epsilon(\mathbf{k})$  in eq. (12). For  $t/U \leq 0.25$  the dispersion function is a minimum at the zone boundary, and attains a maximum value at  $\mathbf{k}=(0, 0)$  and  $(\pi, \pi)$ . A typical result is shown in fig. 1 for  $t/U=0.1$ . The effective mass of the hole is smaller in the direction  $(0, 0)$  to  $(\pi, \pi)$  than in the direction  $(0, \pi)$  to  $(\pi, 0)$ . These results are consistent with previous studies of the  $t$ - $J$  model. For  $t/U \geq 0.25$ , however, new local minima appear at  $(0, 0)$  (or  $(\pi, \pi)$ ) which becomes the absolute minimum when  $t/U$  becomes large enough. An illustrative example is shown in fig. 1b for  $t/U=0.4$ . Again, the same anisotropy of the effective mass of the hole is observed here. The discrepancies with

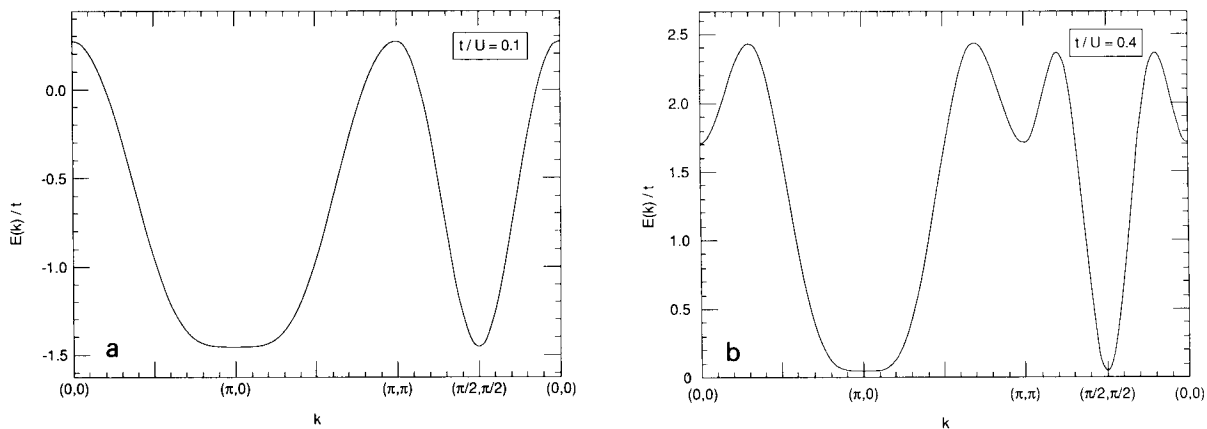


Fig. 1. Dispersion curve,  $\epsilon(\mathbf{k})/t$ , plotted along the direction  $\Gamma M X \Gamma$  for (a)  $t/U=0.1$  and (b)  $t/U=0.4$  (at  $t=1$ ).

previous studies can be attributed to the fact that for  $t/U \geq 0.25$  the  $t$ - $J$  model and Hubbard model are no longer compatible.

The hole energy  $E$ , identified as the bottom of the hole energy band, is plotted in fig. 2 for  $0 \leq t/U \leq 0.5$ . Numerical results for the hole energy from exact diagonalizations of the  $t$ - $J$  model on a  $4 \times 4$  lattice and the Hubbard model on a ten-site lattice [4] are shown as well. (Note that the allowed momenta for the ten-site lattice Hubbard model are  $\mathbf{k} = (3\pi/5, \pi/5)$ ,  $(2\pi/5, 4\pi/5)$  (plus their  $\pi/2$  rotated states),  $(0, 0)$  and  $(\pi, \pi)$  only; so the comparison here is only tentative.) For  $t/U \leq 0.25$  our results agree with the exact diagonalization results of both the  $t$ - $J$  model and the Hubbard model. For  $t/U \geq 0.25$ , in which the  $t$ - $J$  model is no longer compatible with the Hubbard model, our results are still in agreement with the exact diagonalization results of the Hubbard model.

Fig. 3 compares results for the hole bandwidth for  $0 \leq t/U \leq 0.5$ . Note that the bandwidths for both Hubbard model calculations agree very well for  $t/U \leq 0.25$ . The discrepancy which exists for  $t/U \geq 0.25$  may be due to both finite-size effects of the small-size cluster calculations and the need for higher level corrections of the CCA. However, it is clear that the bandwidth for the  $t$ - $J$  model is appreciably smaller than that for the Hubbard model. We believe that the difference comes from the absence of the three-site hopping term in the  $t$ - $J$  model, and is not due to finite-size effects. Although this three-site hopping term is not explicit in the Hubbard model, it is generated in its strong-coupling effective Hamiltonian and is of the same order in  $t/U$  as the  $J$ -term in the  $t$ - $J$  model. Thus, this implies that the  $t$ - $J$  model does not suffice to describe accurately the basic features of the Hubbard model in the strong-coupling limit. A more detailed study of the nearly half-filled strong-coupling Hubbard model by both higher levels of the CCA and exact diagonalization of a larger lattice would definitely give us a clearer picture.

In summary, we have investigated the ground state of a single hole in the half-filled Hubbard model on a 2D square lattice using a reformulation of the coupled-cluster method. In the strong-coupling limit we have obtained an analytical expression of the hole energy dispersion  $\epsilon(\mathbf{k})$  with several of its features consistent with earlier studies of the Hubbard model and  $t$ - $J$  model. An appreciable discrepancy on the hole bandwidth is, however, found between the Hubbard model and the  $t$ - $J$  model. We believe that this discrepancy is due to the absence of the three-site hopping term in the  $t$ - $J$  model. This, in turn, implies that the  $t$ - $J$  model does not suffice to describe accurately the basic features of the Hubbard model in the large Coulomb repulsion limit.

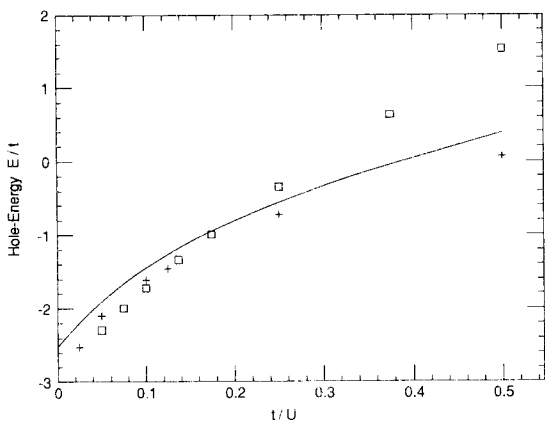


Fig. 2. Hole energy  $E/t$  versus  $t/U$  (at  $t=1$ ). The solid line represents the results from coupled-cluster calculations. Crosses refer to exact diagonalization results of the Hubbard model on a ten-site lattice, whereas squares denote the exact diagonalization results of the  $t$ - $J$  model on a  $4 \times 4$  lattice.

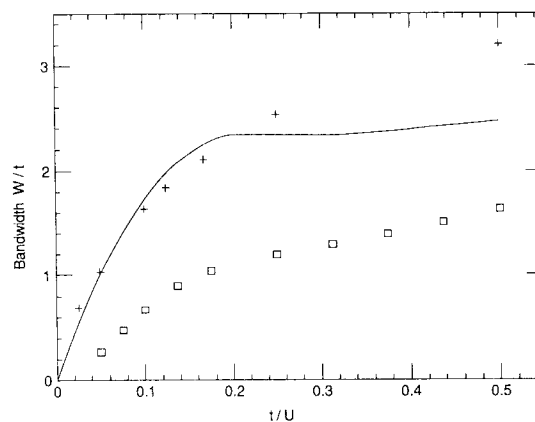


Fig. 3. Bandwidth  $W/t$  versus  $t/U$  (at  $t=1$ ). The solid line represents the results from coupled-cluster calculations. Crosses refer to exact diagonalization results of the Hubbard model on a ten-site lattice, whereas squares denote the exact diagonalization results of the  $t$ - $J$  model on a  $4 \times 4$  lattice.

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### References

- [1] P.W. Anderson, *Science* 235 (1987) 1196.
- [2] B. Shraiman and E. Siggia, *Phys. Rev. Lett.* 61 (1988) 467;  
S. Sachdev, *Phys. Rev. B* 39 (1989) 12232;  
C. Kane, P. Lee and N. Read, *Phys. Rev. B* 39 (1989) 6880;  
S. Trugman, *Phys. Rev. B* 37 (1988) 1597;  
M. Boninsegni and E. Manousakis, preprint.
- [3] E. Kaxiras and E. Manousakis, *Phys. Rev. B* 38 (1988) 866;  
J. Bonca, P. Prelovsek and I. Sega, *Phys. Rev. B* 39 (1989) 7074;  
E. Dagotto, A. Moreo and T. Barnes, *Phys. Rev. B* 40 (1989) 6721;  
W. Stephen, K.J. von Szczepanski, M. Ziegler and P. Horsch, *Europhys. Lett.* 11 (1990) 675;  
V. Elser, D.A. Huse, B.I. Shraiman and E.D. Siggia, *Phys. Rev. B* 41 (1990) 6715.
- [4] E. Dagotto et al., NSF-ITP-89-187, November 1989.
- [5] M. Roger and J.H. Hetherington, *Europhys. Lett.* 11 (1990) 255.
- [6] R.F. Bishop and H.G. Kümmler, *Phys. Today* 40 (3) (1987) 52, and references therein.
- [7] C.F. Lo, E. Manousakis and Y.L. Wang, to be published.
- [8] J. Moré, B. Garbow and K. Hillstom, User guide for MINIPACK-1, Argonne National Labs Report ANL-80-74, Argonne, IL (1980).