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Ground State Properties of the Periodic Anderson Model

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ABSTRACT: The ground state energy, hybridization matrix element, local moment and spin density correlations of a one dimensional, finite chain periodic symmetric Anderson model are obtained using numerical simulations and compared with perturbation theory and strong coupling results. We find that the local f-electron spins are compensated by correlation with other f-electrons as well as band electrons leading to a non-magnetic ground state.

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We have studied the ground state properties of a one-dimensional symmetric periodic Anderson model using stochastic Monte Carlo techniques. Traditionally, the numerical study of the ground state properties of finite quantum spin chains[1] have provided physical insight into the properties of many-body systems. In addition, such results provided a testing ground for approximate techniques such as the Gutzwiller variational approach[2-5] and large orbital degeneracy N^{-1} expansions.[6,7] Usually, these solutions have been obtained by the exact diagonalization of the Hamiltonian using Lanczos-like procedures. In this spirit, Jullian and Martin[8] have used a Lanczos diagonalization to study periodic Anderson model chains. However, the two-orbital periodic Anderson model has 16 states per site so the complexity of the problem restricted their work to the exact diagonalization of 2 and 4-site chains. Here, using Monte Carlo techniques,[9,10] we present results for the ground state properties of chains which are sufficiently large (16 sites) that the bulk limit is sensibly approximated. We analyze these results to determine the effects of the Coulomb interaction on the ground state energy, hybridization matrix element, f-site local moment and the magnetic correlations. We find that the ground state exhibits short range magnetic correlations and that the local f-electron spin moments are compensated by correlations with other f-electrons as well as band electrons leading to a non-magnetic ground state.

The Hamiltonian for the one-dimensional periodic Anderson model can be written as

$$H = \sum_{l\sigma}[-t(d^{\dagger}_{l+1\sigma}d_{l\sigma} + d^{\dagger}_{l\sigma}d_{l+1\sigma}) - V(d^{\dagger}_{l\sigma}f_{l\sigma} + f^{\dagger}_{l\sigma}d_{l\sigma}) + \epsilon_f n^f_{l\sigma} + \frac{U}{2}n^f_{l\sigma}n^f_{l-\sigma}] \qquad (1)$$

Here $d^{\dagger}_{l,\sigma}$ and $f^{\dagger}_{l,\sigma}$ create Wannier electrons in d- and f-like orbitals on site l with spin σ and $n^f_{l\sigma} = f^{+}_{l\sigma}f_{l\sigma}$. The d-orbitals overlap via the hopping term t to form a band. The local f-orbitals with site energy ϵ_f are hybridized through V with the d-orbitals. Two electrons in the same f-orbital experience a Coulomb repulsion U. In the following we treat the particle-hole symmetric case in which $\epsilon_f = -U/2$.

We have used both a modified projector method[9] in which the operator $e^{-\beta H}$ is applied

to project out the ground state and a finite temperature Monte Carlo technique with an exact updating procedure.[10] The projector technique allowed us to achieve large β values ($\beta \sim 10^2$) to check that the ground state properties were being obtained. The finite temperature technique allowed us to see the approach to low temperature, and further results obtained from it will be reported elsewhere.[11,12] Here we discuss the ground state properties.

In the absence of the Coulomb interaction U, Eq. (1) describes a simple two band system with band energies

$$E_k^{\pm} = \epsilon_k/2 \pm \sqrt{(\epsilon_k/2)^2 + V^2} \tag{2}$$

Here $\epsilon_k = -\cos(k)$ for $t = 0.5$. These bands are separated by a gap of 2Δ with $2\Delta = (\sqrt{1+4V^2} - 1)$. In the non-interacting ground state the lower band E_k^- is entirely filled with spin up and spin down electrons giving a ground state energy per site of

$$E_0(0) = \frac{2}{N} \sum_k E_k^- \tag{3}$$

and the system is in a singlet state with $\langle M_z^2 \rangle = 0$ where M_z is the total z-component of spin. As the Coulomb interaction U is turned on, we expect the system to remain in a singlet state unless a phase transition were to occur at some critical value of U. Our numerical results give no evidence for such a transition. Carrying out perturbation theory[13] to order U^2 one finds that the ground state energy per site is

$$E_0(U) = \frac{2}{N} \sum_k E_k^- - \frac{U}{4} - \frac{U^2}{N^3} \sum_{pkq} \frac{v_p^2 u_{p+q}^2 v_{k+q}^2 u_k^2}{E_{k+q}^+ + E_p^+ - E_k^- - E_{p+q}^-} \tag{4}$$

with

$$u_p^2 = \frac{1}{2}(1 + \frac{\epsilon_p}{\sqrt{\epsilon_p^2 + 4V^2}}) \quad v_p^2 = \frac{1}{2}(1 - \frac{\epsilon_p}{\sqrt{\epsilon_p^2 + 4V^2}}) \tag{5}$$

Here the expansion parameter is U/Δ. In the strong coupling limit where U/Δ is large, one has through $0(U^{-1})$,

$$E_0(U) = -\frac{U}{2} + \frac{2}{N}\sum_k \epsilon_k f(\epsilon_k) - \frac{2V^2}{N}\sum_k \frac{1-f(\epsilon_k)}{(U/2+\epsilon_k)} \tag{6}$$

with $f(\epsilon_k)$, the zero temperature Fermi factor equal to 1 for $\epsilon_k < 0$, 0.5 for $\epsilon_k = 0$ and 0 for $\epsilon_k > 0$.

Simulations were carried out for a variety of parameters, with fixed $t = 0.5$. The ground state energy per site is a smooth function of the number of sites N and for $N = 16$ the systematic change with size is inside our statistical error. The values of $E_0(U)/|E_0(0)|$, for $V = 0.375$, corresponding to $\Delta = 0.25$, are plotted versus U in Figure 1. The dashed line is the second order perturbation theory result, Eq. (4), and the solid line is the strong coupling expression Eq. (6). The rms errors are of order the size of the points.

In the presence of U, the effective hybridization is reduced due to the Coulomb correlations. A useful measure of this reduction is given by the ratio of $(f^+_{l\sigma}d_{l\sigma} + d^+_{l\sigma}f_{l\sigma})$ in the interacting ground state to its value when $U = 0$.

$$\frac{\langle f^+_{l\sigma}d_{l\sigma} + d^+_{l\sigma}f_{l\sigma}\rangle}{\langle f^+_{l\sigma}d_{l\sigma} + d^+_{l\sigma}f_{l\sigma}\rangle_0} \tag{7}$$

This matrix element can be directly obtained from E_0 using the Feynman-Hellman relation

$$\langle f^+_{l\sigma}d_{l\sigma} + d^+_{l\sigma}f_{l\sigma}\rangle = \frac{1}{2}\frac{\partial}{\partial V}E_0 \tag{8}$$

The dashed line in Figure 2 was obtained by differentiating the perturbation theory expression for E_0, Eq. (4), with respect to V, while the solid line corresponds to the strong coupling result

$$\langle f^+_{l\sigma}d_{l\sigma} + d^+_{l\sigma}f_{l\sigma}\rangle = -\frac{2V}{N}\sum_k \frac{1-f(\epsilon_k)}{(U/2+\epsilon_k)} \tag{9}$$

obtained from Eq. (6). The points were calculated from the simulation. One clearly sees the decrease in the effective hybridization as U increases. Since the gap varies as the square

of the hybridization matrix element, it has decreased by a factor of 10 for U of order 3. For the symmetric Anderson model $\langle n_\sigma^f \rangle$ remains fixed at 0.5, and thus in the particle-hole symmetric case the renormalization of the hybridization does not arise[2,3] from a change in $\langle n_\sigma^f \rangle$.

In addition to altering the hybridization, the suppression of charge fluctuations by the Coulomb interaction leads to the formation of local moments on the f-orbitals. A measure of this is the average of the square of the f-orbital single site magnetization $m_z^f(l) = n_{l\uparrow}^f - n_{l\downarrow}^f$.

$$\langle m_z^f(l)^2 \rangle = 1 - 2\langle n_{l\uparrow}^f n_{l\downarrow}^f \rangle \tag{10}$$

For $U = 0$, $\langle n_{l\uparrow}^f n_{l\downarrow}^f \rangle = \frac{1}{4}$ and $\langle m_z^f(l)^2 \rangle$ is equal to 0.5. For large U, double occupancy is reduced by the Coulomb repulsion and $\langle m_z^f(l)^2 \rangle$ approaches 1. Again the derivative of the ground state with respect to U provides a convenient way of evaluating this. With $\epsilon_f = -U/2$,

$$\langle m_z^f(l)^2 \rangle = -2 \, \frac{\partial E_0}{\partial U} \tag{11}$$

For weak coupling, Eq. (4) gives

$$\langle m_z^f(l)^2 \rangle = 0.5 + \frac{4U}{N^3} \sum_{pkq} \frac{v_p^2 u_{p+q}^2 v_{k+q}^2 u_k^2}{E_{k+q}^+ + E_p^+ - E_k^- - E_{p+q}^-} \tag{12}$$

and for strong coupling we have from Eq. (6),

$$\langle m_z^f(l)^2 \rangle = 1 - \frac{2V^2}{N} \sum_k \frac{1 - f(\epsilon_k)}{(U/2 + \epsilon_k)^2} \tag{13}$$

These are plotted as the dashed and solid curves, respectively, in Figure 3, which shows $\langle m_z^f(l)^2 \rangle$ versus U. The points were obtained from the simulation.

These results clearly show that U reduces the hybridization and produces local moments on the f-orbitals. In addition, it leads to interactions between these moments and the d-electrons. In order to explore this feature we have calculated various magnetic and

charge density correlation functions. The charge density correlations show the suppression produced by U. The magnetic correlation functions $\langle m_z^f(l)m_z^f(0)\rangle$ and $\langle m_z^d(l)m_z^f(0)\rangle$ with $m_z^d(l) = n_{l\uparrow}^d - n_{l\downarrow}^d$ and $m_z^f(l) = n_{l\uparrow}^f - n_{l\downarrow}^f$, respectively, were found to exhibit short range correlations which act to screen the f-orbital moment. This is clearly seen in Figure 4, where they are plotted for the first few spacings for $U/\Delta = 2.0$.

To see how the magnetic correlations act to screen the f-site moments leading to a singlet ground state, we consider the total z-component of magnetization.

$$M_z = m_z^f(0) + \sum_{l=1}^{N-1} m_z^f(l) + \sum_{l=0}^{N-1} m_z^d(l) \tag{14}$$

If the ground state expectation value of M_z vanishes, then squaring Eq. (14) and taking its ground state expectation value leads to a compensation sum rule

$$\langle m_z^f(0)^2\rangle = -\sum_{l=1}^{N-1}\langle m_z^f(l)m_z^f(0)\rangle - \sum_{l=0}^{N-1}\langle m_z^d(l)m_z^f(0)\rangle \tag{15}$$

Using the correlation functions shown in Figure 4 to evaluate the left-hand side of Eq. (15) gives 0.65 ± 0.02, while $\langle (m_z^f(0))^2\rangle = 0.64 \pm 0.02$. Thus, just as in the single magnetic impurity case, the f-moment is compensated by correlations in the surrounding medium.[14] However, as discussed by Nozieres,[15] in the periodic Anderson model this compensation does not arise from just the d-band electrons. Rather, as one sees in Figure 4, an important part arises from the $f - f$ magnetic correlations.

Conclusion: Simulations of the symmetric 1-D periodic Anderson model show that the Coulomb interaction leads to a reduction in the f-d hybridization, local moment formation on the f-orbitals and short-range magnetic moment correlations resulting in a singlet ground state. The ground state energy as well as the hybridization matrix element $\langle f_{l\sigma}^+ d_{l\sigma} + d_{l\sigma}^+ f_{l\sigma}\rangle$ and the mean square local f-moment $\langle m_z^f(l)^2\rangle$ smoothly cross over from the weak coupling to the strong coupling limit. Similar results were found for a variety of parameter values leading us to the conclusion that this type of behavior is a general property of the 1-D symmetric periodic Anderson model.

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FIGURE CAPTIONS

Fig. 1. The ground state energy $E_0(U)/|E_0(0)|$ versus U. Here $t = 0.5$, $V = 0.375$ and $\Delta = 0.25$. The dashed curve corresponds to the second order perturbation theory result Eq. (4), and the solid line is the strong-coupling approximation Eq. (6).

Fig. 2. The hybridization matrix element $\langle f_{l\sigma}^{+} d_{l\sigma} + h.c. \rangle$ normalized to its $U = 0$ value versus U for the same parameters as in Figure 1. The dashed curve is the second order perturbation theory result, and the solid line is the strong-coupling limit.

Fig. 3. The square of the f-orbital single site magnetization $\langle (m_l^f)^2 \rangle$ versus U for the same parameters as in Figure 1.

Fig. 4. The $\langle m_z^f(l) m_z^f(0) \rangle$ and $\langle m_z^d(l) m_z^f(0) \rangle$ magnetic correlation functions versus site separation l for $U/\Delta = 2.0$.

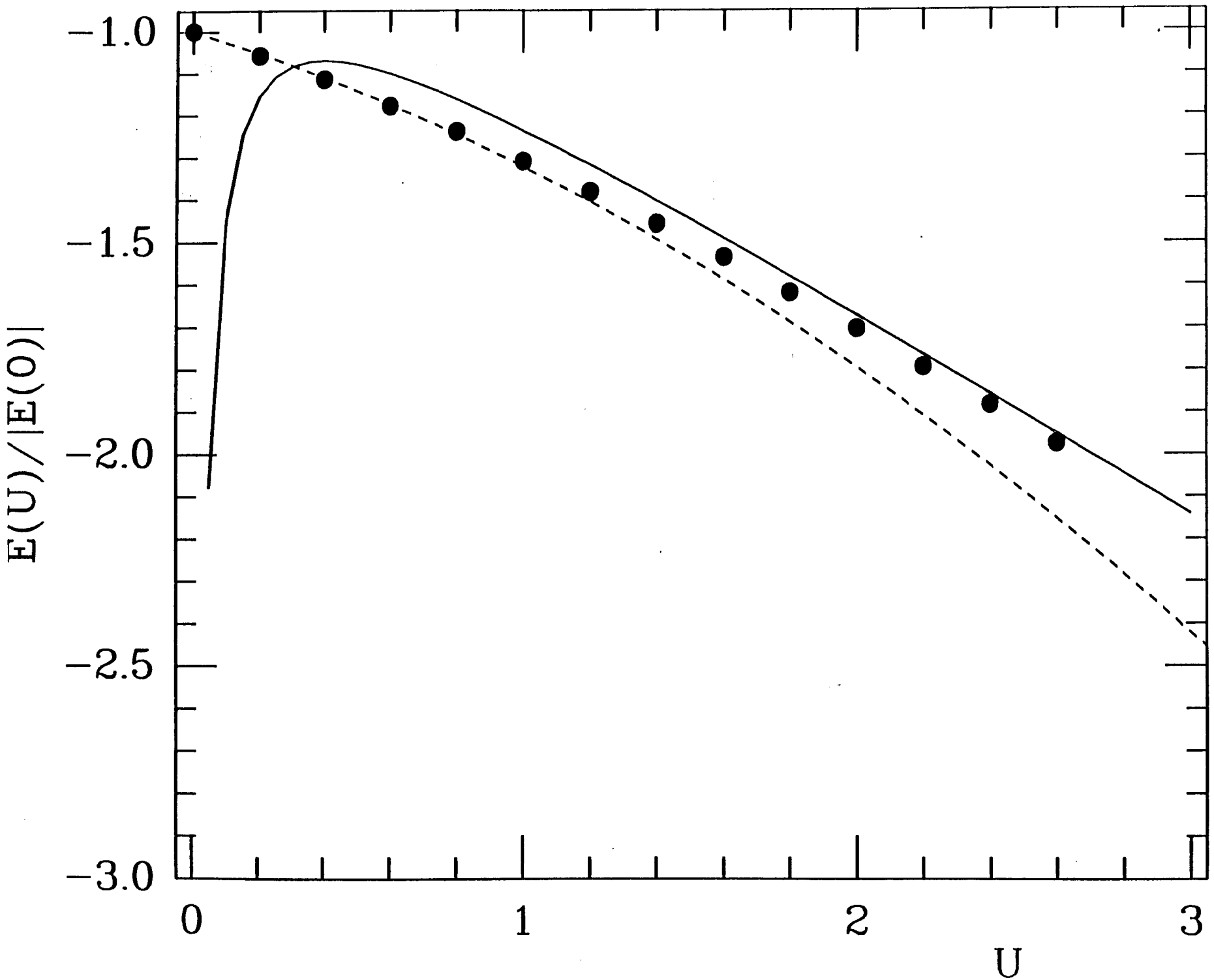


Fig. 1

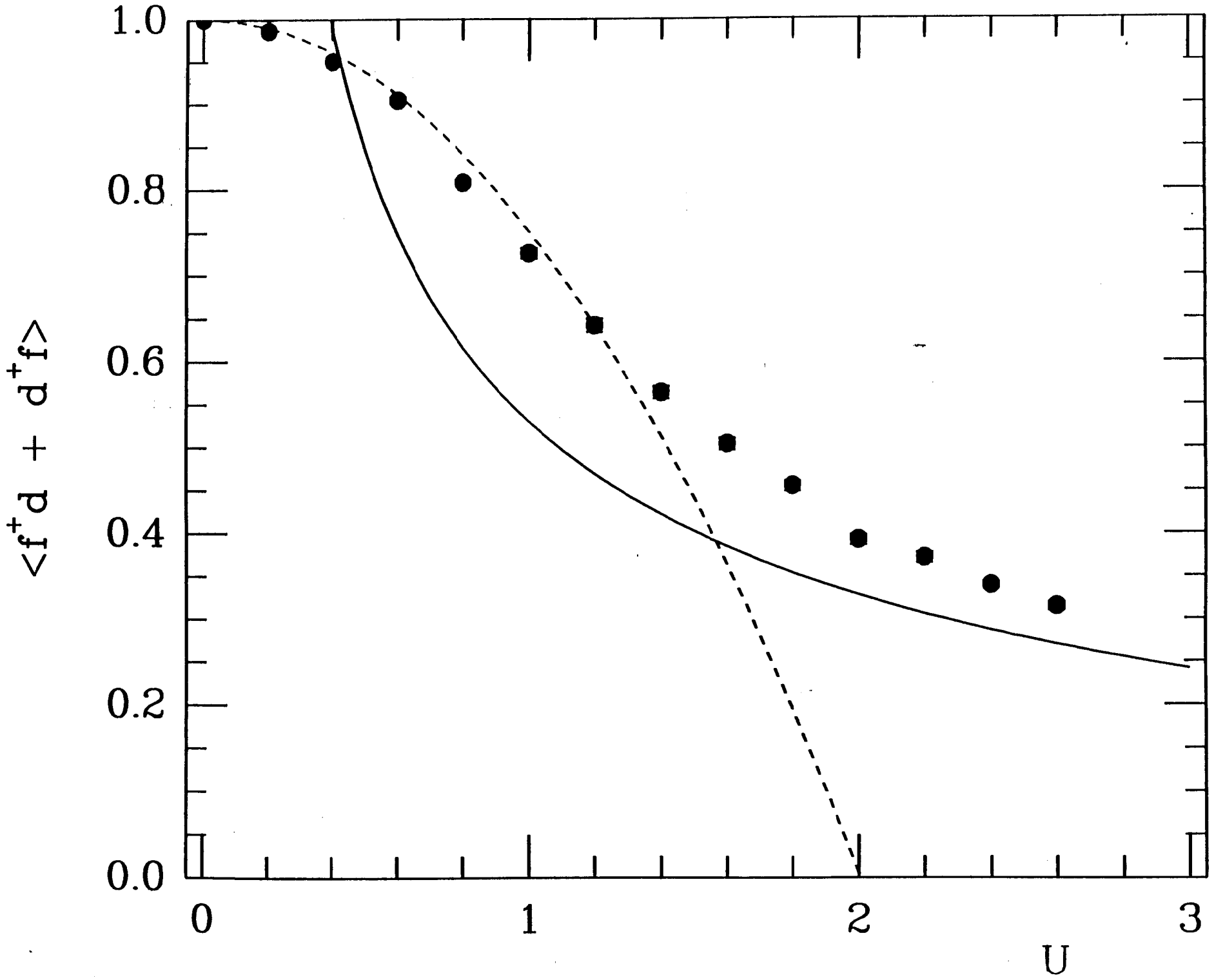


Fig. 2

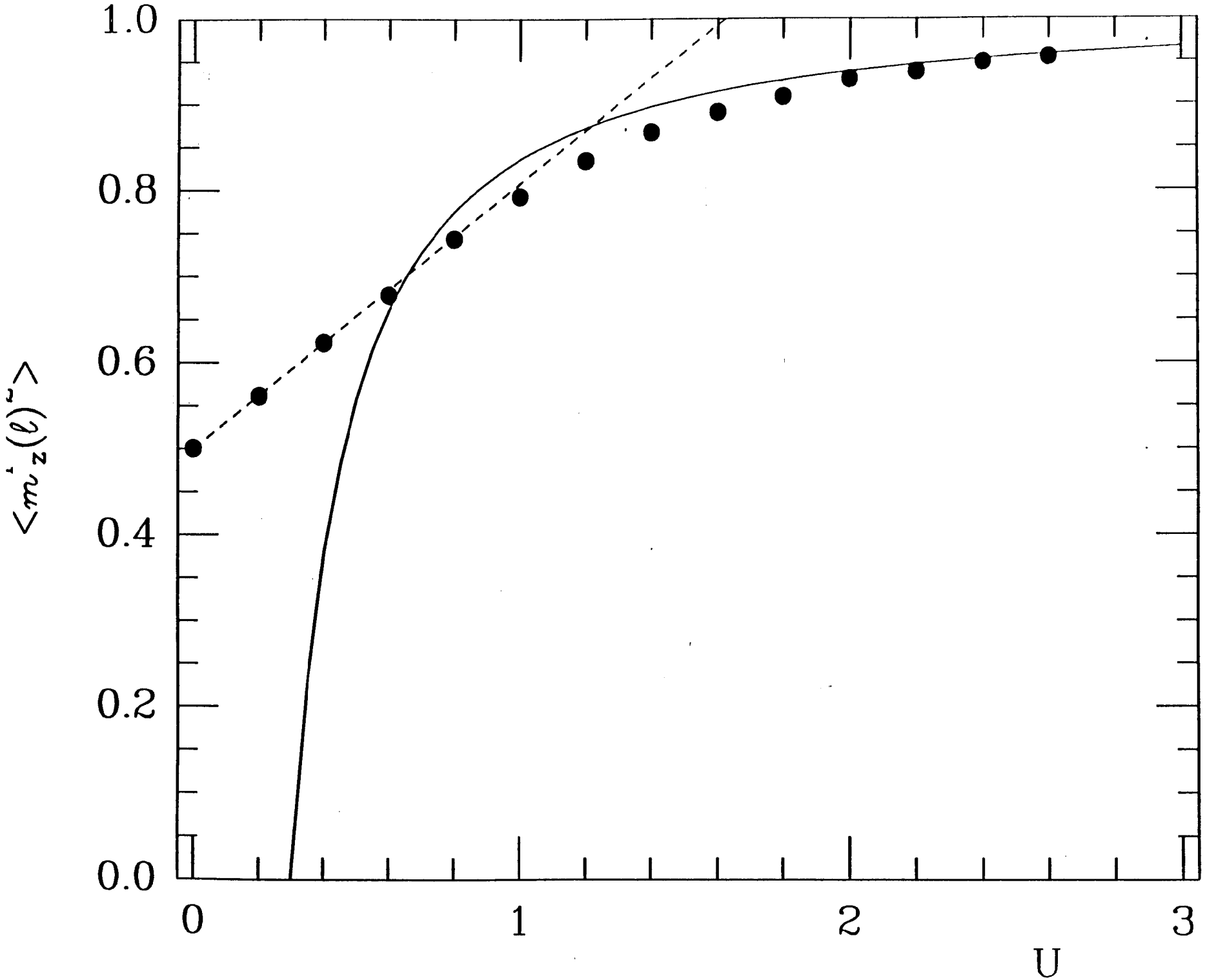
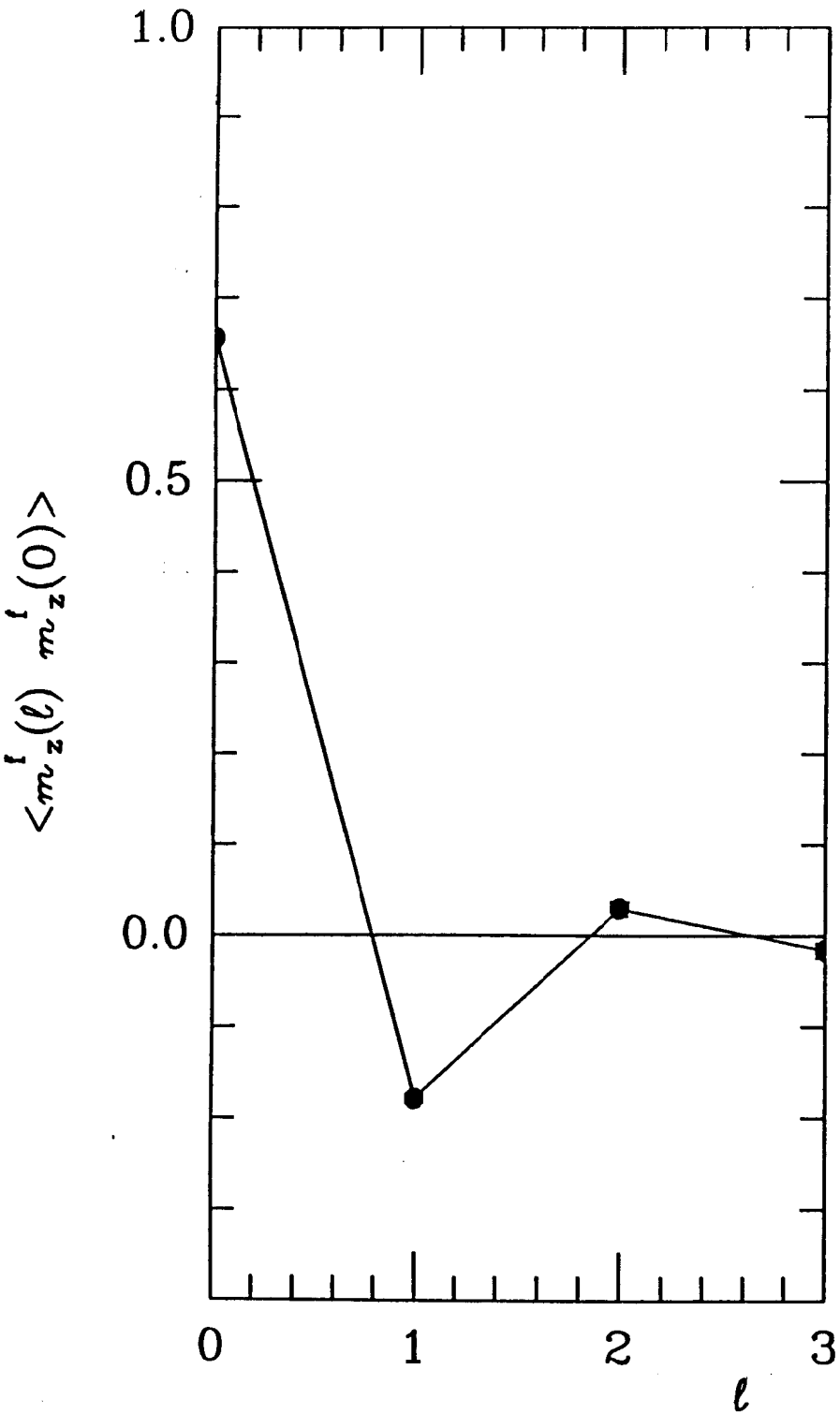


Fig. 3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2
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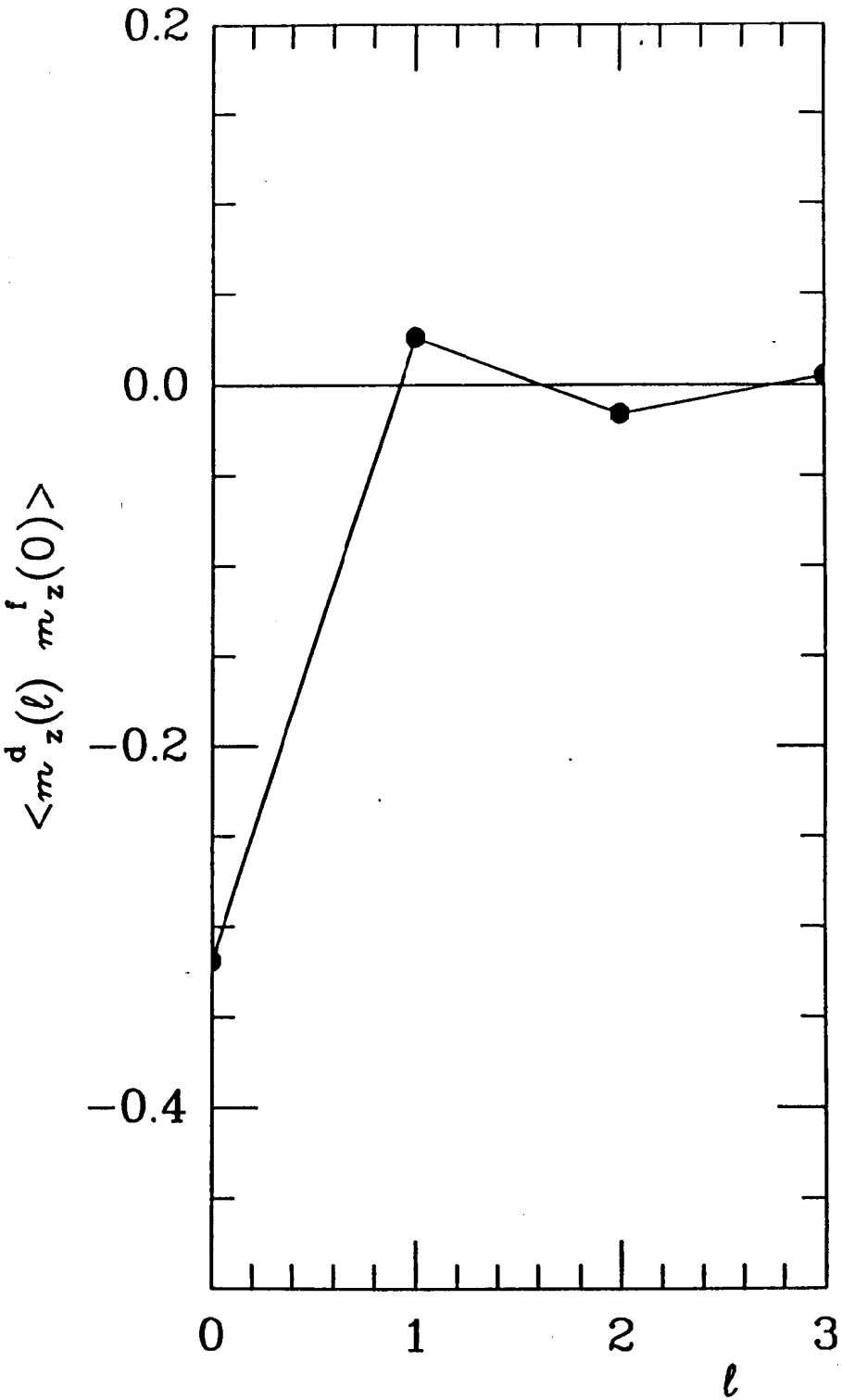
$\langle m^t_z(\ell)\ m^t_z(0)\rangle$


0.2
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−0.2
−0.4
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1
2
3
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$\langle m^d_z(\ell)\ m^t_z(0)\rangle$

Fig. 4