AD-A265 648

②

IMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. AGENCY USE ONLY *(Leave blank)*

2. REPORT DATE
May 1993

3. REPORT TYPE AND DATES COVERED
professional paper

4. TITLE AND SUBTITLE
INFINITE VOLUME EXTRAPOLATIONS OF FINITE CLUSTER CALCULATIONS—HOW CORRECT ARE THESE

5. FUNDING NUMBERS
In-house funding

6. AUTHOR(S)
S. Mazumdar, F. Guo, D. Guo, K-C Ung, J. T. Gammel

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Naval Command, Control and Ocean Surveillance Center (NCCOSC)
RDT&E Division
San Diego, CA 92152-5001

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
Naval Command, Control and Ocean Surveillance Center (NCCOSC)
RDT&E Division
San Diego, CA 92152-5001

10. SPONSORING/MONITORING AGENCY REPORT NUMBER

DTIC
ELECTE
JUN 10 1993
S D
E

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release; distribution is unlimited.

12b. DISTRIBUTION CODE

13. ABSTRACT *(Maximum 200 words)*

Extrapolations of numerical data obtained from finite cluster calculations to the infinite volume limit can often give incorrect results. We discuss four separate cases: (a) the intensity of the lowest two-photon absorption in the infinite polyene, (b) bond alternation in the infinite polyene; (c) Cooper type pairing in the simple Hubbard model, and (d) pairing within the extended Hubbard model.

93 2

93-12971

Published in *Proceedings*, Discussion meeting on Strongly Correlated Electron Systems in Chemistry (SPRINGER), January 1993.

14. SUBJECT TERMS
superconductivity

15. NUMBER OF PAGES

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	SAME AS REPORT

21a NAME OF RESPONSIBLE INDIVIDUAL J. T. Gammel	21b TELEPHONE *(Include Area Code)* (619) 553-6576	21c OFFICE SYMBOL Code 573

INFINITE VOLUME EXTRAPOLATIONS OF FINITE CLUSTER CALCULATIONS, —HOW CORRECT ARE THESE?

S. Mazumdar, F. Guo, D. Guo, and K. -C. Ung
Department of Physics, University of Arizona
Tucson, AZ 85721, USA

J. Tinka Gammel
Materials Research Branch, NCCOSC RDT&E Division
San Diego, CA 92152-5000, USA

ABSTRACT

Extrapolations of numerical data obtained from finite cluster calculations to the infinite volume limit can often give incorrect results. We discuss four separate cases: (a) the intensity of the lowest two-photon absorption in the infinite polyene, (b) bond alternation in the infinite polyene, (c) Cooper type pairing in the simple Hubbard model, and (d) pairing within the extended Hubbard model.

I. Introduction

Approximate analytic techniques have been known to lead to qualitatively incorrect predictions for solid state systems with strong electron correlation. Exact numerical techniques are therefore often employed to determine the behavior of such systems. This approach consists of two steps, the first of which involves an exact calculation for a finite cluster. The second step involves an extrapolation of the finite cluster data to the thermodynamic limit. We point out that extrapolations are not always valid, and in certain cases can lead to erroneous theoretical predictions.

We believe that there is a strong necessity for such a discussion currently. The technique of using exact numerical data for finite systems to determine the behavior in the solid began with the classic calculations for the Heisenberg chain by Bonner and Fisher[1], who, however, emphasized the necessity of having one dimension and short range interaction. In recent years, however, the numerical approach has been employed more and more liberally, and calculations are routinely being done for higher dimensions, as well as for Hamiltonians with long range interactions. Our hope is that the present work will lead to more systematic studies of finite size effects.

We discuss four specific cases here. The correct solutions to these problems are of interest to chemists and physicists. These four different cases demonstrate different finite size effects, and in each case we show that literal interpretation of finite cluster calculations predict *qualitatively* incorrect result.

II. Exact Finite Cluster Calculations

A. The intensity of the two-photon absorption (TPA) to the $2A_g$ and other low lying A_g states in the infinite polyene The occurrence of the lowest two-photon state, the $2A_g$, below[2] the lowest one-photon state, the $1B_u$ (note that optically inactive B_u states need not be considered), in finite polyenes necessarily requires a correlated description for the π-electrons[2,3]. The entire discussion of TPA has. however, so far been limited to the energy of the $2A_g$ state. Here we extend this discussion to the question of the intensity of the TPA to the $2A_g$ (and other low lying A_g states) as a function of the chain length N.

This discussion will be in the context of the extended Hubbard Hamiltonian,

$$H = t\sum_{i,\sigma}[1-(-1)^i\delta](c^+_{i,\sigma}c_{i+1,\sigma} + c^+_{i+1,\sigma}c_{i,\sigma})$$
$$+U\sum_i n_{i,\uparrow}n_{i,\downarrow} + V\sum_i (n_i - 1)(n_{i+1} - 1) \qquad (1)$$

where all operators and parameters have their usual meanings. We begin with the $U = V = 0$ limit. In Fig. 1 we show the occupancies of the highest two valence band levels and lowest two conduction band levels for the $1A_g$ (the ground state), the $1B_u$, the $2A_g$ and the $2B_u$ for arbitrary N. TPA is given by the third order nonlinearity $\chi^{(3)}(-\omega;\omega,\omega,-\omega) \equiv \chi^{(3)}_{TPA}$,

$$\chi^{(3)}_{TPA} = \sum_{j,k,l}\frac{\langle 1A_g|\mu|jB_u\rangle\langle jB_u|\mu|kA_g\rangle\langle kA_g|\mu|lB_u\rangle\langle lB_u|\mu|1A_g\rangle}{(\omega_{jB_u}-\omega)(\omega_{kA_g}-2\omega)(\omega_{lB_u}-\omega)} + \cdots \qquad (2)$$

where μ is the dipole operator. Conventional wisdom has been that TPA occurs every time an energy denominator goes to zero in Eq.(2). We show below that this is not true.

The intensity of the TPA to the $2A_g$ was calculated exactly for $U = V = 0$ and for N = 6, 8, 10 and 12, typical chain lengths for which calculations are done for nonzero U and V. As seen in Fig. 2., TPA intensity increases with N here, suggesting a large finite TPA intensity for $N \to \infty$. This, however, is incorrect.

The model in Eq. (1) has charge-conjugation symmetry, which implies that for every single-particle valence band level at energy $-\epsilon$ there exists a conduction band level at ϵ. In the infinite chain, dipole allowed absorptions occur only between these symmetrically placed molecular orbitals, in agreement with k-conservation. Thus for TPA to any intraband A_g state, only two "symmetric" B_u states need be considered. For the $2A_g$, these two B_u states are the $1B_u$ and the $2B_u$. For any N, the absolute values of the transition dipole moments $\langle 2A_g|\mu|1B_u\rangle$ and $\langle 2A_g|\mu|2B_u\rangle$ are equal, while because of the fermion character of the electron the products $\langle 1A_g|\mu|1B_u\rangle\langle 1B_u|\mu|2A_g\rangle$ and $\langle 1A_g|\mu|2B_u\rangle\langle 2B_u|\mu|2A_g\rangle$ are of opposite signs. At $N \rightarrow \infty$, these two products become equal in magnitude, while having opposite signs. This implies that the contribution to $\chi^{(3)}$ in Eq.(2) by the $2A_g$ vanishes[4], and the TPA intensity to the $2A_g$ and other band edge two-photon states is zero for $N \rightarrow \infty$.

We emphasize that the above analysis does not imply a zero intensity for the total TPA to intraband two-photon states. Even with the restriction to "symmetric" B_u states, there can be very weak TPA due to relatively high energy A_g states that are slightly removed from the band edge. For example, one can have such a high energy intraband A_g state that is coupled to the $1B_u$ and a B_u state that requires excitation from deep inside the valence band to deep inside the conduction band. Because of the small nonzero energy difference between the two B_u states now, the cancellation is no longer total. Weak TPA to states away from the band edge is expected, and explains the shift of the TPA to higher energy from the optical band edge in the long chain[5]. Nevertheless, at infinite N, TPA to band edge two-photon states goes to zero, in contradiction to the prediction form Fig. 2. Since calculations of correlated chains are limited to the region where TPA increases with N, the integration of these two contradictory results is an important issue.

For the noninteracting case TPA can be calculated for arbitrary N. In Fig. 3 we show the TPA intensity to $2A_g$ as a function of N. It is seen that the TPA intensity does go to zero at very large N, but only after a maximum is reached. Thus calculations near $N = 10$ predict qualitatively incorrect results. On the other hand, once the mechanism is understood, one can probe the N-dependence of $|S^-/S^+|$, where S^- and S^+ are the negative and positive contributions to the TPA. This is shown in Fig. 4, where the expected N-dependence is observed.

We are now in a position to calculate TPA to $2A_g$ in long correlated chains. We have adopted the novel configuration interaction (CI) approach of Srinivasan and Ramasesha[6] for the interacting Hamiltonian of Eq. (1), with a cutoff 4t in the energies of single-particle configurations. The approach can give the $2A_g$ below the $1B_u$ even in long chains. In Table 1 we compare calculated $|S^-/S^+|$ for many different U, V and δ. The ratio cannot be 1 in N = 20 - 30, but comparisons with the noninteracting cases strongly suggest that the TPA to the $2A_g$ should be very weak in the long chain limit even for nonzero Coulomb interaction, in contrast to what would be predicted from exact evaluation[7] of the TPA near $N = 10$. This prediction is in agreement with the tiny TPA to $2A_g$ in poly-BCMU polydiacetylene[8], and the noted absence of the two-photon resonance in β-carotene[9].

B. The bond-alternation problem in the one dimensional half-filled band

Within the Su-Schrieffer-Heeger Hamiltonian,

$$H = \sum_{i,\sigma}[t - \alpha(y_i - y_{i+1})](c^+_{i,\sigma}c_{i+1,\sigma} + c^+_{i+1,\sigma}c_{i,\sigma}) + \frac{1}{2}\kappa\sum_i(y_i - y_{i+1})^2 \quad (3)$$

bond-alternation in the infinite polyene is unconditional. Coulomb interactions can enhance this bond alternation. For long range Coloumb interactions H_{ee} of the form ,

$$H_{ee} = U\sum_i n_{i,\uparrow}n_{i,\downarrow} + \sum_{i,j} V_j(n_i - 1)(n_{i+j} - 1) \quad (4)$$

two sharp inequalities give the ground state broken symmetry[10]. For off-site Coulomb parameters that obey the convexity condition, $V_{j+1}+V_{j-1} > 2V_j$, the ground state can only be a bond-order wave (BOW) with alternating bonds or a charge density wave (CDW) with a periodic modulation of the on-site charge density. The dominant broken symmetry is given by the inequality,

$$\sum V_{2n+1} \lessgtr \frac{1}{2}U + \sum V_{2n} \tag{5}$$

where a smaller left hand side (LHS) gives BOW, while a smaller right hand side (RHS) gives a CDW. All Pariser-Parr-Pople (PPP) parametrizations for the infinite polyene then predict enhanced BOW[10].

The approach involving extrapolation technique was also employed in this case, by Ramasesha and Soos[11]. These authors calculated the electronic energy gained for fixed bond alternation, when compared to the equal bond length case, for open even chains, closed $N = 4n$ rings, and closed $N = 4n + 2$ rings, and extrapolated the energy gains in the three series against $1/N$ for the PPP-Ohno Hamiltonian. Enhanced energy gains compared to the simple Hückel case was taken to be the proof of enhanced BOW. While the result for the carbon-based polymers agrees with the prediction from Eq. (5), let us examine this approach in detail.

The extrapolation of the 4n-ring series is invalid, since the RHS of Eq. (5) in this case always has an extra term that precludes the CDW entirely and guarantees enhanced BOW. The even chain extrapolation has many different finite size effects. First, even chains have an odd number of bonds, thus precluding equal bond lengths for small N. Second, the range of the Coulomb interaction within PPP models is longer than the N for which calculations are being done. This leads to a different Hamiltonian for each N. Finally, real space many-electron configurations have entirely different matrix elements of H_{ee} within the open chain boundary condition and for the periodic ring. For example, the configuration ...20202020..., where the numbers denote site-occupancies, has a matrix element $4U - 8V_1 + 8V_2 - 8V_3 + 4V_4$ in the ring, but the matrix element is $4U - 7V_1 + 6V_2 - 5V_3 + 4V_4 - 3V_5 + 2V_6 - V_7$ in the open chain. This last difference shifts the boundary between the BOW and the CDW considerably, such that the open chain would predict enhanced BOW even as Eq. (5) predicts a CDW. Since the $4n + 2$ ring series can only have a few data points, this makes the extrapolation technique itself suspect.

We demonstrate the above by doing the open chain calculation for the PPP-Ohno parameters corresponding to polysilane. It has been assumed that this has a simple BOW ground state with very large alternation[12]. We choose a U of 9.04 eV and evaluate V_j from the PPP-Ohno relationship,

$$V_j = \frac{U}{[1 + 0.39R_j^2]^{1/2}} \tag{6}$$

where the R_j are the distances between the polysilane "sites", and are taken from literature[12]. Eq. (5) predicts a CDW, with different charge densities on the orbitals on the same silicon atom. The extrapolation technique nevertheless predicts enhanced BOW, as seen in Fig 5.

Our motivation here was to demonstrate the inapplicability of the extrapolation technique for the bond alternation problem and not to claim that polysilane is a CDW. Whether or not polysilane is a CDW depends on whether the PPP-Ohno model is truly appropriate for polysilanes. It is, however, interesting to note that the occurrence of the lowest two-photon absorption considerably above the lowest one-photon absorption[13] occurs naturally within the CDW model.

C. Pairing in Hubbard models A great deal of numerical effort has gone into investigating whether pairing of the Cooper type occurs in the weakly doped two-dimensional Mott-Hubbard insulator. More recently, such a pairing mechanism has been proposed[14] for doped C_{60}. The two dimensional calculations have now been extended to the case of weakly coupled layers[15]. Specifically, these calculations involve determination of the ground state energies of the half-filled band system, and the electronic energies needed to add one and two electrons (holes). Pairing is supposed to occur if the quantity

$$\Delta E = 2E(N+1) - E(N) - E(N+2) \tag{7}$$

is positive. In spite of considerable effort, it is still not entirely clear whether pairing occurs in two dimension or not, or what the actual mechanism of pairing is in the various cases.

We focus here on the mechanism of the pairing, and what this says about pairing in the infinite system. Fye et al[16] showed that pairing of the above kind is not limited to two or three dimension, but can also occur in one dimensional periodic rings with $N = 4n$ atoms. The limitation to 4n rings is very suggestive, as small 4n-rings undergo Jahn-Teller distortions. In Fig. 6 we show our results of the pairing calculations for N = 4 and 8. The pairing disappears for the Jahn-Teller distorted rings. To understand this better, we calculated the effect of the Hubbard U on the Jahn-Teller distortion of the 4n and $4n-1$ electron systems. These results are shown in Fig. 7. It is seen that U strongly reduces the gain in energy for the Jahn-Teller distortion of the even (4n) electron system, but the distortion of the odd numbered (4n -1) electron system remains virtually unaffected. This then gives us the mechanism of the pairing. The information regarding the tendency to distort is built into the wave function in the form of the various bond order parameters. By not letting the system distort, we are overestimating the energies in each case, but as Fig. 7 indicates, this overestimation is much stronger for the odd electron case than for the even electron case. The calculated energy required to add one hole (or electron) to the undistorted system is therefore too high, thereby giving "pairing".

This same mechanism can explain "pairing" in higher dimension. In Fig. 8 we show the results of our calculation for the simple cube, and for various distorted forms. For the undistorted simple cube, we merely reproduce the results of White et al.[17], — two distinct regions are found in which pairing is seen to occur. For the cube stretched along one axis, we see that the pairing still exists. This is not the Jahn-Teller mode for the cube, the noninteracting limit still having degeneracies. However, the pairing at small U has disappeared for both the Jahn-Teller distorted cube as well as the structure with all three hopping integrals different. This clearly indicates the relationship between pairing and the degeneracies in the single particle limit. We have once again calculated the effect of the correlation parameter U on the Jahn-Teller distortions . The result is identical to that in Fig. 7, the tendency to distort is almost unaffected for the 7 electron system, but for the 6 electron system this is strongly suppressed. The mechanism of pairing at small U in the cube is then the same as in the 4n ring. In the absence of distortion, the energy to add one hole or electron is being overestimated.

We have repeated such calculations for a number of three dimensional molecules, and have found the following. For an N site system, pairing at small U occurs only if the $(N-1)$ (or $(N+1)$) electron system has a strong tendency to have a Jahn-Teller distortion. Thus the mechanism of pairing at small U in all these case is related to the suppression of Jahn-Teller distortion. Since the Jahn-Teller distortion results from the discrete level degeneracies in finite molecules, we conclude that the observed pairing in in the small U region in similar calculations is a finite size effect.

Fig. 8 explains the oscillation in the pairing energy of the cube. Pairing at large U is unrelated to the tendency to have Jahn-Teller distortion. We have occasionally found such pairing at large U also in other systems, though not necessarily accompanied by pairing at small U. The occurrence of such large U pairing in nonbipartite systems (for e.g., in a pentagonal prism) indicates that this is also unrelated to antiferromagnetism. Currently we are investigating whether the large U pairing is also a finite size effect, and if so, the nature of the finite size effect. The present work indicates the absence of pairing in the two dimensional Hubbard model, as well as in weakly coupled layers.

D. Pairing due to intersite interactions Many calculations exist that find a pairing driven by intersite interactions rather than the on-site Coulomb interaction. Since the intersite interactions in these calculations are different, it is impossible to give a general critique. Nevertheless, we believe numerical calculations here would in most cases find phase segregation, rather than simple pairing, if adequate numbers of electrons or holes are added to the half-filled band. In the case of the t-J model, this tendency to phase segregate has been discussed[18]. We choose one simple example, a calculation claiming pairing driven by the nearest neighbor Coulomb interaction[19] in the two-dimensional quarter-filled band, to illustrate our point.

For large U and V, the quarter-filled band is a CDW. The configuration with one extra particle is as shown in Fig. 9. This has configuration interaction with a higher energy configuration which is at energy 2V relative to it. If, however, one adds two particles which occupy neighboring empty sites in the CDW, the lowest energy configuration has configuration interaction with a configuration that is at an energy V relative to it. Thus, CI should give pairing in two dimension, though not in one dimension. This was actually numerically demonstrated by Mazumdar and Ramasesha[19]. The fallacy in this argument becomes clear once three particles are added to the system as shown in Fig. 9 Now, the lowest energy configuration has CI with a configuration at the same energy, so that a cluster of three particles is favored over a cluster of two and an isolated particle. Similar qualitative arguments favor phase segregation in related models. Thus, once again, thus, the pairing found within such calculations is a finite size effect.

III. Conclusions

The major conclusion of this presentation is that there are many different finite size effects, and even when a given approach is satisfactory for the determination of one property of a given class of materials (e.g., the energy of the $2A_g$ in the infinite conjugated polyene), it does not necessarily mean that the same approach is satisfactory for other properties (in this case ground state bond alternation and the intensities of TPA). Finite size effects should be investigated for each different problem separately. Probably the most useful approach to avoid the pitfalls is to have a physical and intuitive mechanism of the effect in question in mind. However, this can hardly be prescribed as a general approach. One simple way to investigate finite size effects is to carefully investigate the size dependence of the property in question within the noninteracting model, for which calculations can be done for arbitrary sizes. Even though this procedure is simple (and an obvious step), finite correlated clusters are often compared to the infinite noninteracting system, simply because the latter is understood. Such a procedure can, and often does, erroneously ascribe effects due to finite size to correlations.

Acknowledgement

Work at Arizona was supported by NSF grant No. ECS-89-11960. J. T. Gammel was supported by a NRC-NRaD Research Associateship through a grant from the ONR and the DOE.

REFERENCES

1. J. C. Bonner and M. E. Fisher, *Phys. Rev.* **135**, A640, (1964).
2. B. S. Hudson, B. E. Kohler, and K. Schulten, *Excited States* 6, edited by E. C. Lim, (Academic, New York) (1982).
3. K. Schulten, I. Ohmine, and M. Karplus, *J. Chem. Phys.* 64, 4222, (1976).
4. Dandan Guo, S. Mazumdar, S. N. Dixit, *Nonlinear Optics*, (1993).
5. G. P. Agrawal, C. Cojan, and C. Flytzanis, *Phys. Rev. B* 17, 776, (1978).
6. B. Srinivasan and S. Ramasesha, *Solid State Commun.* 81, 831, (1992).
7. Z. G. Soos and S. Ramasesha, *J. Chem. Phys.* 90, 1067, (1989).
8. W. E. Torruellas, K. B. Rochford, R. Zanoni, S. Aramaki, and G. I. Stegeman, *Opt. Commun.* 82, 94, (1991).
9. J. B. van Beek, F. Kajzar, and A. C. Albrecht, *J. Chem. Phys.* 95, 6400, (1991).
10. S. Mazumdar and D. K. Campbell, *Phys. Rev. Lett.* 55, 2067, (1985).
11 Z. G. Soos and S. Ramasesha *Phys. Rev. B* 29, 5410, (1984).
12. R. G. Kepler and Z. G. Soos, *Phys. Rev. B* 43, 12530, (1991).
13. J. R. G. Thorne, Y. Ohsako, R. M. Hochstrasser, and J. M. Zeigler, *Chem. Phys. Lett.* **162**, 455, (1989).
14. S. Chakravarty, M. P. Gelfand, and S. Kivelson, *Science* 254, 970, (1991).

15. D. G. Kanhere, in present proceedings.

16. R. M. Fye, M. J. Martins, and R. T. Scalettar, *Phys. Rev. B* **42**, 6809, (1990).

17. S. R. White, S. Chakravarty, M. P. Gelfand, and S. A. Kivelson, *Phys. Rev. B* **45**, 5062, (1992).

18. V. J. Emery, S. A. Kivelson, and H. Q. Lin, *Phys. Rev. Lett.* **64**, 475, (1990).

19. S. Mazumdar and S. Ramasesha, *Synth. Metals* **27**, A105, (1988).

Table Caption

Table 1. The ratio of the negative and positive contributions to the $2A_g$ TPA in long polyene chains within the extended Hubbard model.

Figure Caption

Figure 1. The single-particle orbital electron occupancies of the $1A_g$, $1B_u$, $2A_g$ and the $2B_u$. Only the highest (lowest) two valence (conduction) band levels are shown. All other valence (conduction) band levels are filled (empty).

Figure 2. The intensity of the $2A_g$ TPA in short finite chains within the Hückel model. Here E_g is the $1B_u - 1A_g$ gap. Notice that the intensity increases with N.

Figure 3. The intensity of the $2A_g$ TPA as a function of N within the Hückel model. TPA goes to zero at $N \rightarrow \infty$.

Figure 4. The ratio of the negative and positive contributions to the $2A_g$ TPA as a function of N within the Hückel model.

Figure 5. The electronic energy difference per site between dimerized and the equal bond length even chains for the parameters of Eq. (6). The extropolated $N \rightarrow \infty$ values lies above the value for the dimerized infinite Hückel ring.

Figure 6. Pair binding energies (see Eq. (7)) for the (a) $N = 4$ and (b) $N = 8$ rings. In each case the solid curve corresponds to the undistorted ring, the dashed curve to the Jahn-Teller distorted ring.

Figure 7. The gain in electronic energy on Jahn-Teller distortion for the $N = 4$ ring, as a function of Hubbard U. The solid and dashed curves correspond to the 4 and 3 (5) electron cases respectively.

Figure 8. Pair binding energies in the simple cube and three distorted forms. (i) - - - - - -, simple cube; (ii) ———, stretched cube, $t_1 = t_2 > t_3$; (iii) —

— —, Jahn-Teller distorted cube; (iv) — - — -, all three hopping integrals different. Notice absence of pairing at small U for cases (iii) and (iv).

Figure 9. Quarter-filled extended Hubbard CDW with (a) one extra particle, (b) two extra particles, (c) three extra particles (crosses are particles, dots empty sites). CT excitation in (a) costs energy $2V$, in (b) V, and zero in (c).

Table 1

N	U	V	δ	$\lvert S^-/S^+\rvert$
20	0	0	0.3	0.79
20	3	0	0.3	0.80
20	6	0	0.3	0.78
20	4	1	0.3	0.81
20	0	0	0.1	0.21
20	6	0	0.1	0.67
20	4	1	0.1	0.60
24	0	0	0.3	0.86
24	4	0	0.3	0.85
24	8	0	0.3	0.92
24	4	1	0.3	0.86

Table 1, Mazumdar et al

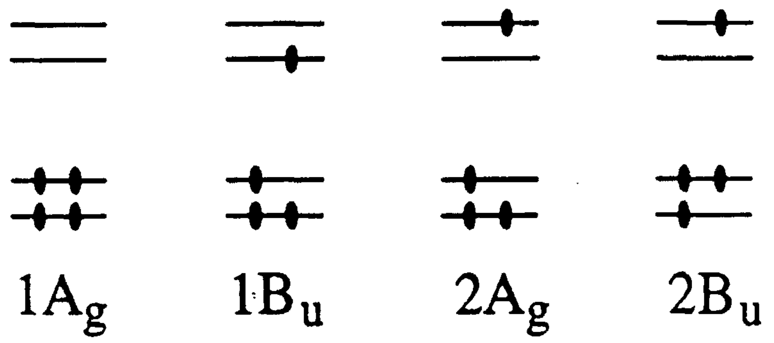

Fig. 1 Mazumdar et al

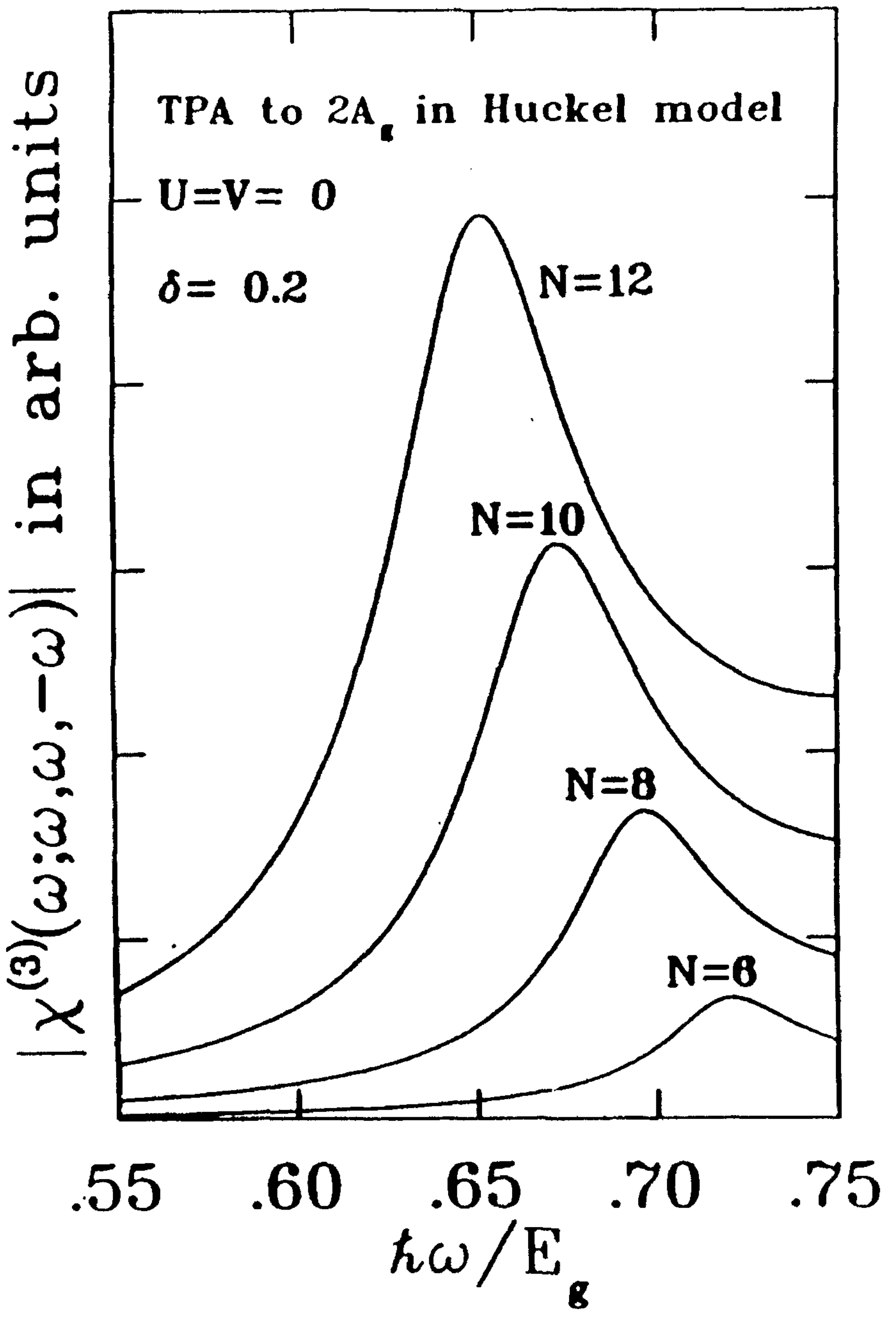

Fig. 2, Mazumdar et al.

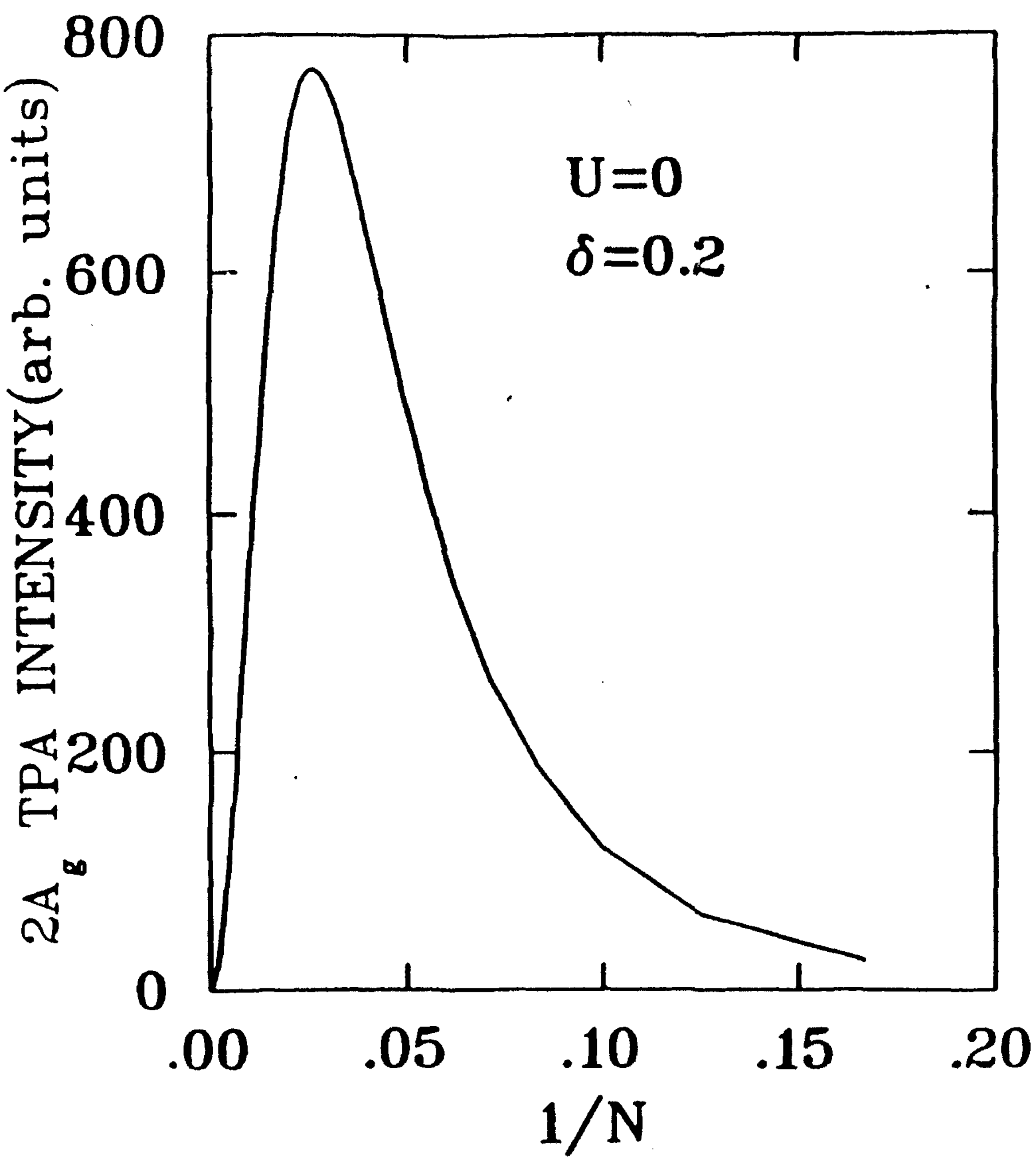

Fig 3 Mazumdar et al

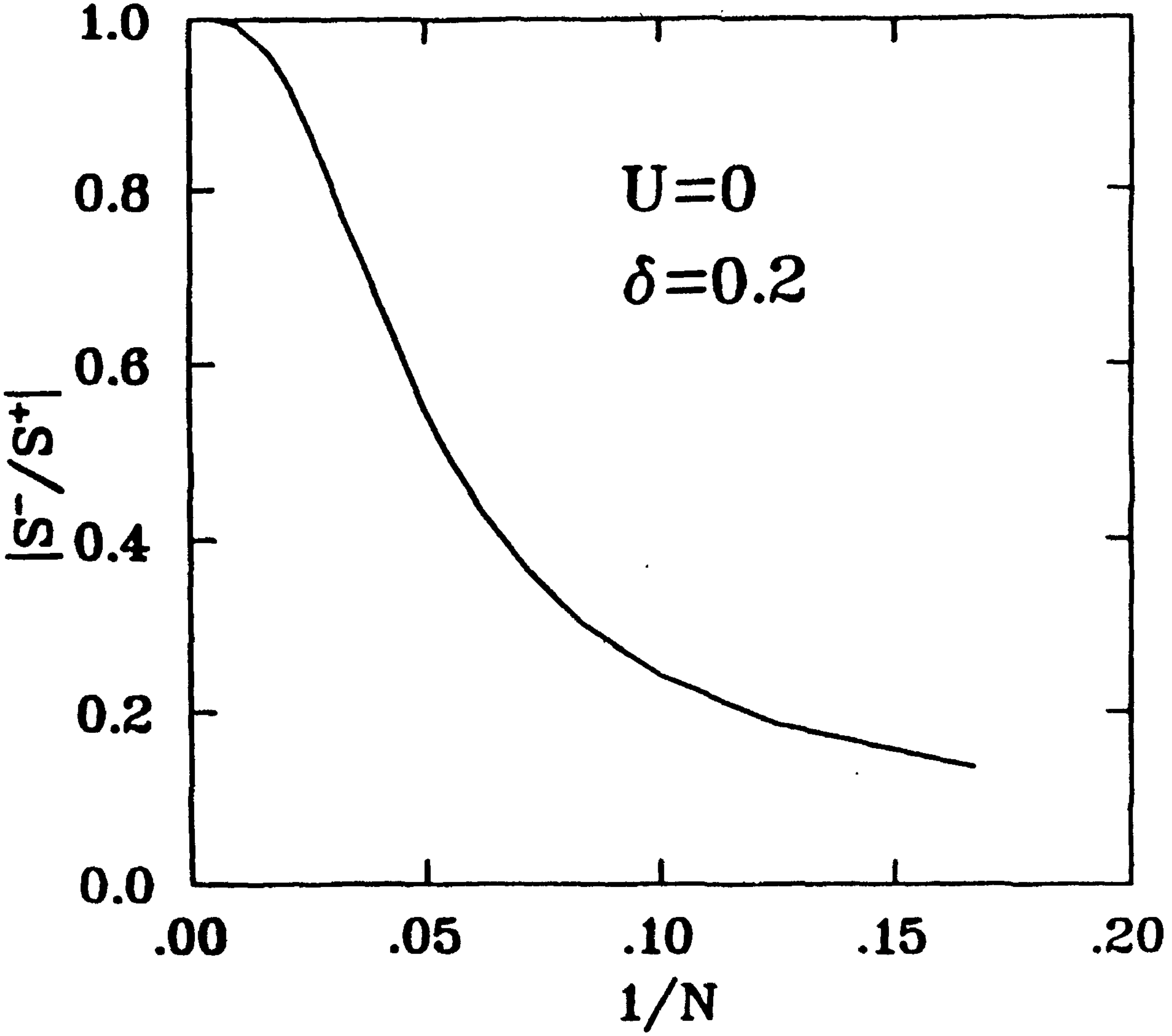

Fig 4, Mazumdar et al

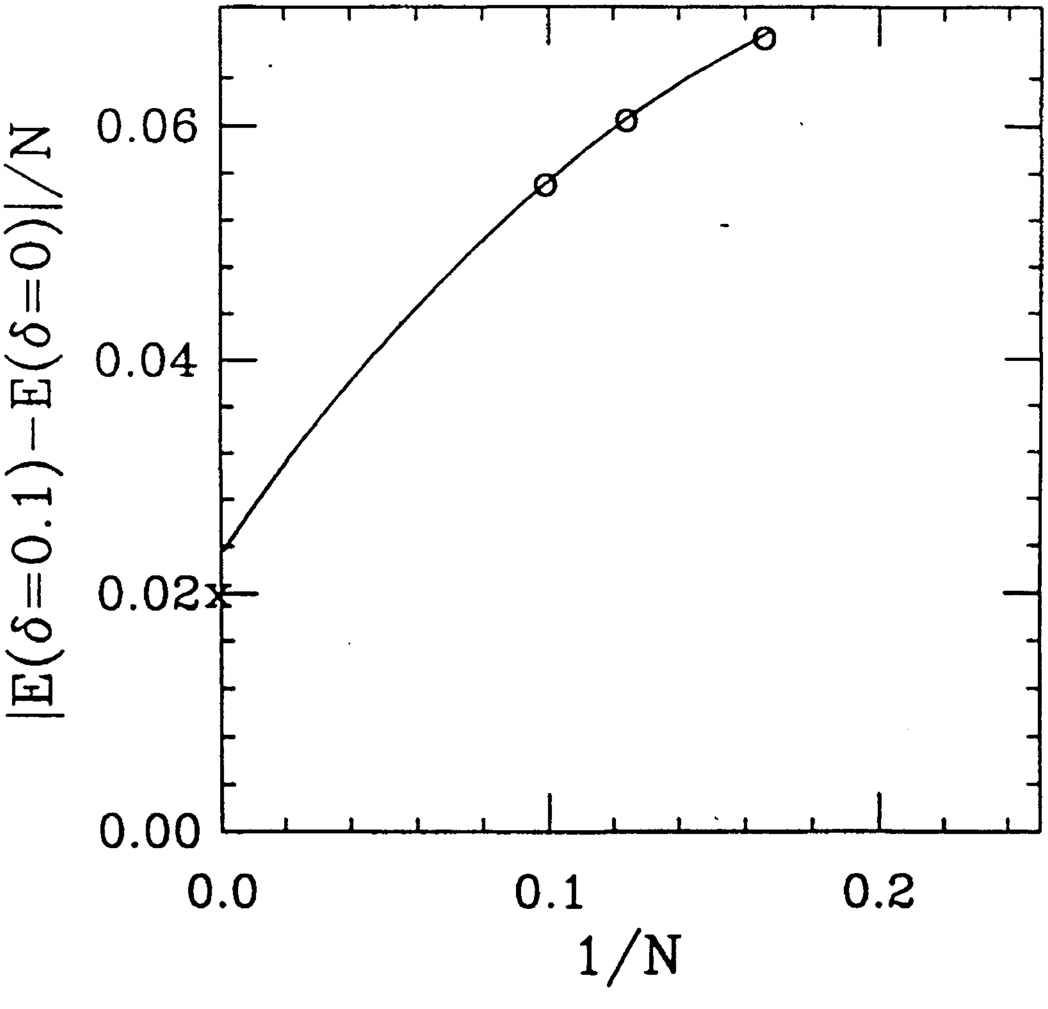

Fig 5. Mazumdar et al.

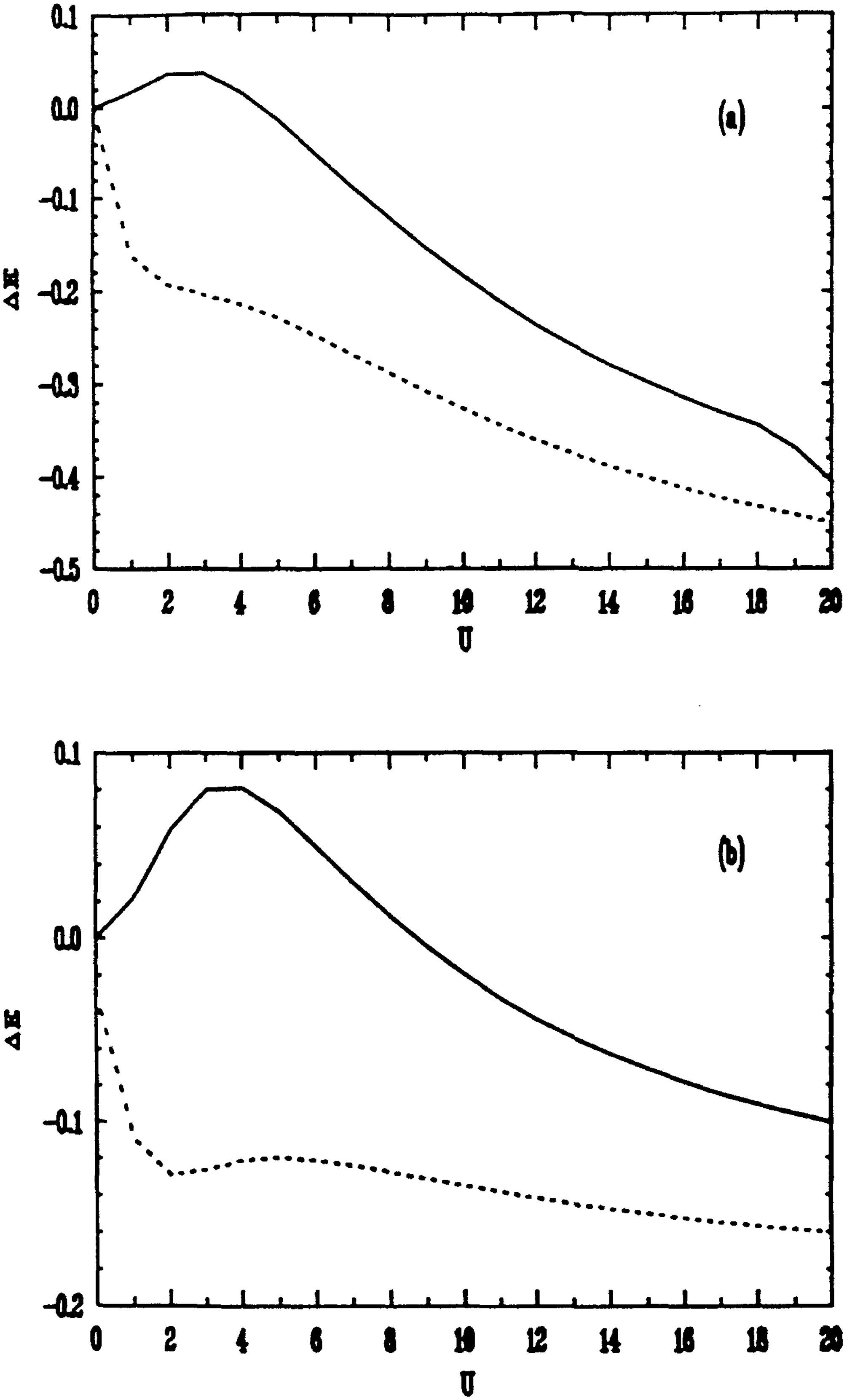

Fig. 6, Mazumdar et al.

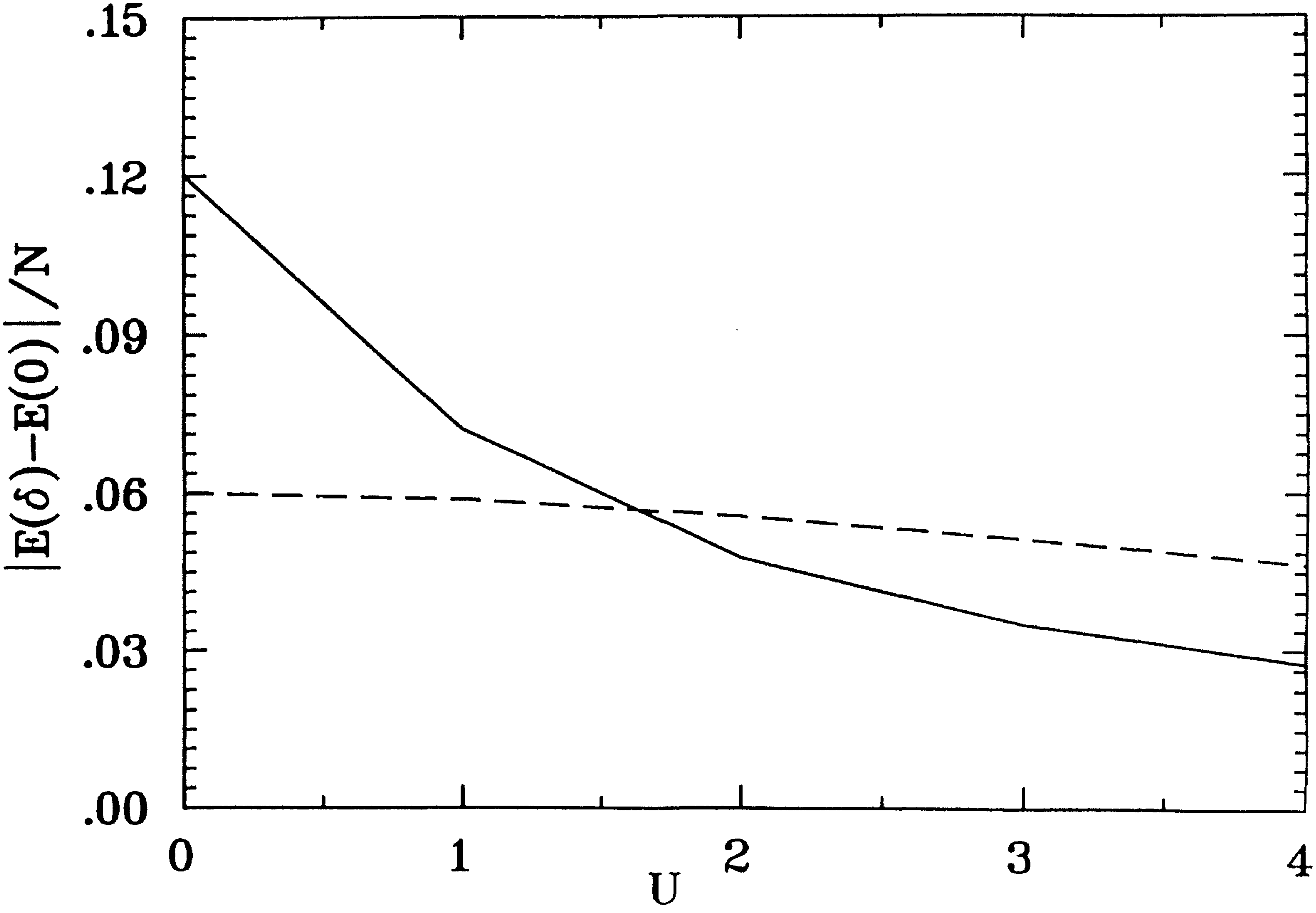

Fig. 4 Mazumdar et al.

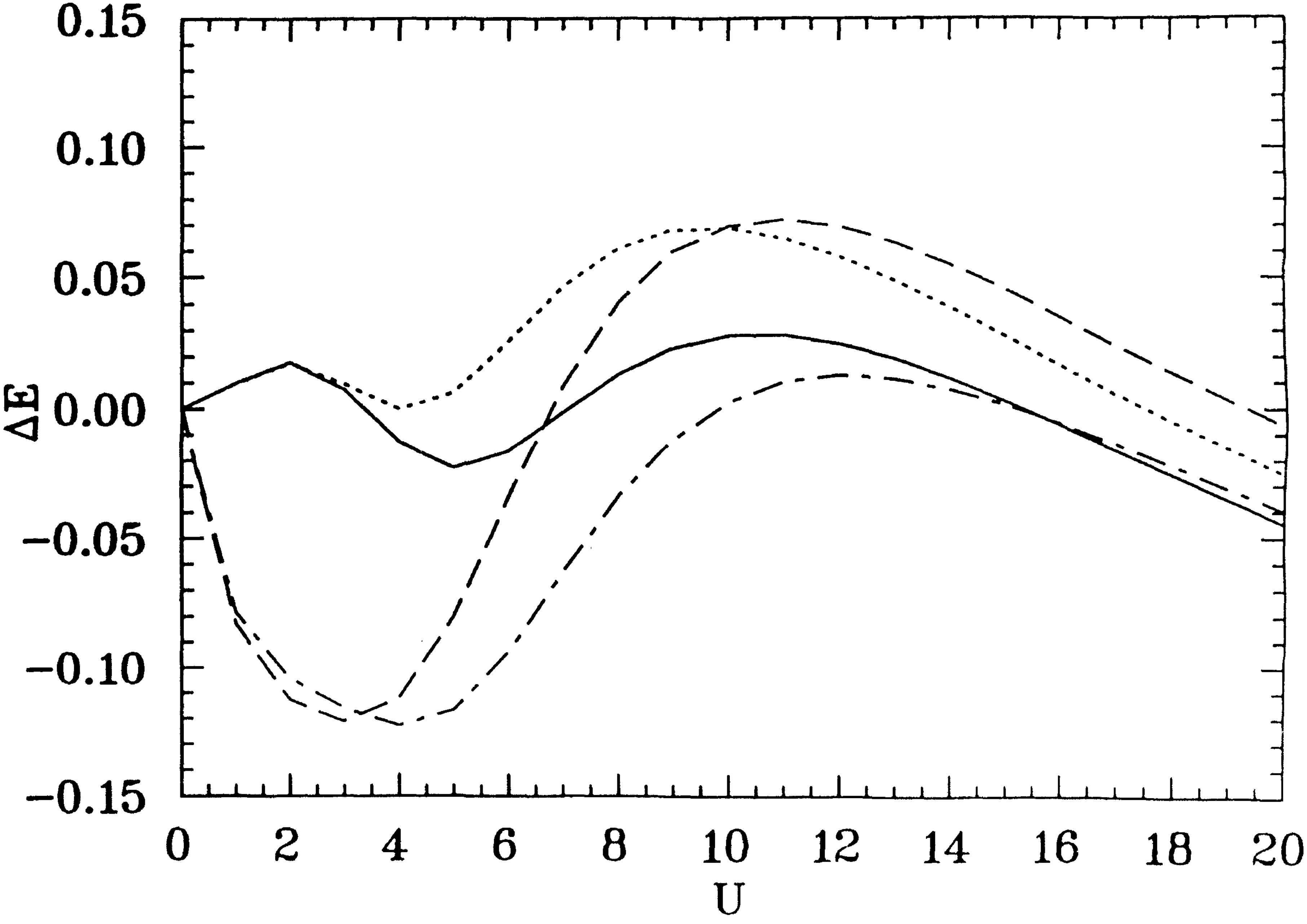

Fig 8 Mazumdar et al.

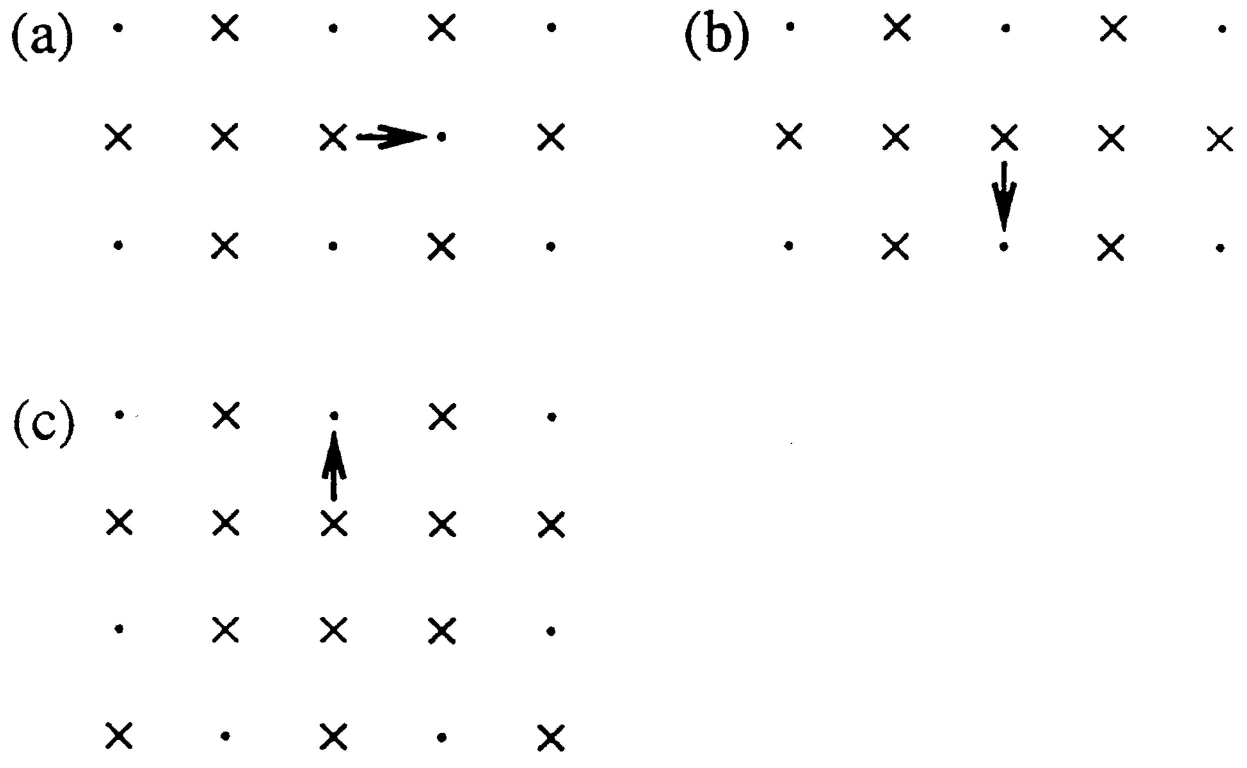

Fig. 9, Mazumdar et al.