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An Extension of the Krieger-Li-Iafrate approximation to the optimized-effective-potential method

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(November 11, 1999)

Abstract

The Krieger-Li-Iafrate approximation can be expressed as the zeroth order result of an unstable iterative method for solving the integral equation form of the optimized-effective-potential method. By pre-conditioning the iterate a first order correction can be obtained which recovers the bulk of quantal oscillations missing in the zeroth order approximation. A comparison of calculated total energies are given with Krieger-Li-Iafrate, Local Density Functional, and Hyper-Hartree-Fock results for non-relativistic atoms and ions.

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I. INTRODUCTION

The optimized-effective-potential method (OEPM) [14] minimizes the Hartree-Fock (HF) configuration average total energy expression given wavefunctions computed in a single central field potential V(r).

$$\frac{\delta E}{\delta V(r)} = \sum_m \int dr' \frac{\delta E}{\delta \phi_m(r')} \frac{\delta \phi_m(r')}{\delta V(r')} = 0 \tag{1.1}$$

This variational expression results in a linear Fredholm integral equation of the first kind for the exchange potential

$$\int dr' K(r,r') V_x(r') = Q(r) \tag{1.2}$$

where the exchange potential is defined as the diference over the classical Hartree potential in V(r). Explicit expressions for the kernal $K(r,r')$ and inhomogenous drive term $Q(r)$ and their properties are supplied in Appendix A. For simplicity we limit ourselves in this paper to non-relativistic systems, the generalization to relativistic systems is straightforward.

By definition the OEPM total energies are closer to Hartree-Fock than parametetric potential model results (e.g. [3]) (which can be viewed as a minimization with a constrained form for V(r) [7]) or by employing wavefunctions obtained from density functional (DF) theories, either directly into the Hartree-Fock energy expression or by using the density functional expression for the total energy explicitly. Fig. (1) presents such a comparison for the ground state configuration of all ionstages for all light elements $Z \leq 36$.

The main disadvantage of the OEPM over DF methods is that at each iterative step of the self-consistent field solution an updated exchange potential must be obtained by constructing and solving Eq. (1.2). The additional computational labour can be seen as arising from discretizing the integral equation into a linear system of N equations in N unknowns, where N, the number of radial mesh points, must be kept modest for speed and memory considerations.

Additionally, some specific features of the kernal imposes special consideration. Solutions to Eq. (1.2) are defined only up to an additive constant determined by boundary conditions.

A discretizion of the integral equation requires that an adequate asymptotic form must be obtained by the last mesh point, before numerical instabilities from the singular nature of the kernal set in. In practice this is often not the case. Furthermore, in practice quadratic forms for the exchange potential near the origin must also be imposed to avoid numerical 'ringing' [4]. These instabilities, arising from the fact that the eigenvalues of the singular value decompostion of the kernal have an accumulation point at zero, implies that small errors in the in-homongenous drive term of the integral equation are amplified in the solution. This instability precludes straight-forward iterative techniques for the solution of the integral equation, a difficulty often plagued by Fredholm integral equations of the first kind unless some sort of regularization is imposed [6].

Alternative approaches to the OEPM (e.g. [7]) have employed multi-dimensional optimizations of the HF energy functional directly. Besides the computational expense of the multi-dimensional optimization, this proceedure requires the concomittent expense of invoking the wave equation solver at each step of the optimization, and the process is usually more time consuming than 'brute-force' discretization of the OEPM integral equation.

To avoid these problems, an approximate solution to the integral equation, the Krieger-Li-Iafrate (KLI) approximation [13], can be employed. Its implementation requires a matrix inversion of dimension of the number of occupied orbitals, is not restricted to modest radial mesh sizes, and has the proper asymptotic form built in. Its disadvantage is that quantal 'bumps' in the exchange potential (as manifested by numerical solutions of the integral equation) are not fully reproduced, the concomittant degradation in the quality of the total energies and wavefunctions are the subject of this investigation.

In this paper we present an extension of the KLI approximation, which retains the aspects of speed and simplicity of the original algorithm, and obtains the bulk of the missing quantal oscillations. It is essentially a pre-conditioning of the first order iterate in an attempted iterative solution of the integral equation, with the KLI solution forming the zeroth order. The utility of this scheme lays in the quality of the first order results, it is not a systematic approach to an iterative solution, for further iterations will exhibit instabilities and diverge from the numerical solution.

II. THE KLI APPROXIMATION AS ZEROTH ORDER ITERATE

The OEPM integral equation can be re-written as

$$\sum_m n_m \omega_m(r)\phi_m(r) = 0 \tag{2.1}$$

where

$$\omega_m(r) = \int_0^\infty dr' \{V_x(r')\phi_m(r') - h_m(r')\} G_m(r,r') \tag{2.2}$$

with the Green's function G_m and Fock term h_m defined as in Appendix A. Note that by definition we have the orthogonality property

$$\langle \omega_m \phi_m \rangle = 0 \tag{2.3}$$

where for simplicity of notation we have adopted the notation

$$\langle f \rangle = \int_0^\infty dr f(r) \tag{2.4}$$

for any radial function f(r). By operating on Eq. (2.1) with $-\partial^2/\partial r^2$ and manipulating we can obtain

$$\sum_m n_m \{\phi_m(r)[\hat{P}_m \omega_m(r)] - \Omega_m(r)\} = 0 \tag{2.5}$$

where

$$\Omega_m(r) = 2\frac{\partial}{\partial r}\left[\omega_m(r)\frac{\partial \phi_m(r)}{\partial r}\right] \tag{2.6}$$

$$\langle \Omega_m \rangle = 0 \tag{2.7}$$

Because ω_m has the property

$$\hat{P}_m \omega_m(r) = p_m(r) \equiv \mu_m(r) - \langle \mu_m \phi_m \rangle \phi_m(r) \tag{2.8}$$

$$\mu_m(r) \equiv V_x(r')\phi_m(r') - h_m(r') \tag{2.9}$$

a straight-forward re-arrangement of Eq. (2.5) leads to

$$V_x(r) = V^S(r) + V^\Omega(r) + \frac{\sum_m n_m \phi_m^2(r)[\langle\langle V_x\rangle\rangle_m - \langle X\rangle_m]}{\sum_m n_m \phi_m^2(r)} \tag{2.10}$$

where in Eq. (2.10) we have introduced the constants

$$\langle\langle V_x\rangle\rangle_m = \int_0^\infty dr V_x(r)\phi_m^2(r) \tag{2.11}$$

$$\langle X\rangle_m = \int_0^\infty dr \phi_m(r) h_m(r) \tag{2.12}$$

and utilized Slater's [1] average-Fock-approximation (AFA) to the exchange potential

$$V^S(r) = \frac{\sum_m n_m \phi_m(r) h_m(r)}{\sum_m n_m \phi_m^2(r)} \tag{2.13}$$

and introduced

$$V^\Omega(r) = \frac{\sum_m n_m \Omega_m(r)}{\sum_m n_m \phi_m^2(r)} \tag{2.14}$$

Slater's AFA is a solution to the OEPM integral equation when the Green's function is approximated [2] by neglecting the orbital dependence of the energy denominator in Eq. (A14).

The KLI approximation is a result of approximating the exact weak constraint

$$\int_0^\infty dr \Omega_m(r) = 0 \tag{2.15}$$

by the strong constraint $\Omega_m(r) = 0$ in Eq. (2.10). (An aternative derivation of the KLI formalism has been given by Nagy [8]. As V_x is undetermined to within a constant we take as boundary condition

$$V_x(r \to \infty) \approx V^{S[0]}(r \to \infty) \tag{2.16}$$

which exhibits for isolated ions the proper exchange hole Coulomb tail. This boundary condition implies that $\langle\langle V_x\rangle\rangle_m = \langle X\rangle_m$ for the least bound orbital, while the other constants

$\langle\langle V_x\rangle\rangle_m - \langle X\rangle_m$ (for m $\neq$ least bound) are determined by solving the number-of-orbitals minus one dimensional system of linear equations formed from taking the expectation value of V_x (the left hand side of Eq. (2.10)) over each orbital.

The results of the KLI approximation are in good agreement with numerical solutions of the integral Eq. (2.1), V_x in the far-field region it exhibits an asymptotic ionic Coulomb exchange hole tail, while in the nea-field region it enters the nucleus with zero slope, properties not possesed by the proto-typical density functional exchange potential

$$V_x(r) = -2\left(\frac{3}{\pi}\rho(\vec{r})\right)^{1/3} \tag{2.17}$$

However quantal oscillations found in the numerical solutions are not properly reproduced by the KLI approximation (Fig. (2)).

III. CORRECTIONS TO THE KLI APPROXIMATION

An iterative proceedure can now be formulated, where given an approximation to the exchange potential (e.g. starting with the KLI result, which is close to the 'exact' OEPM exchange potential) and substituting back into Eqs. (2.2) , one can then calculate an improved estimation of the corrective functions $\Omega_m(r)$ and thereby obtain an improved approximation to the exchange potential

$$\Delta V_x(r) = V_x^{new}(r) - V_x^{old}(r) = V^{\Omega}(r) + \frac{\sum_m n_m\phi_m^2(r)\langle\langle\Delta V_x\rangle\rangle_m}{\sum_m n_m\phi_m^2(r)} \tag{3.1}$$

Note that Eq. (3.1) must be solved as was Eq. (2.10) with the same boundary condition.

Up to this point the KLI approximation (besides avoiding a large matrix solution of the OEPM integral equation) did not require the Green's function explicitly. To proceed with the numerical implementation of an iterative solution we require a computational realization of the Green's function, and this is presented in Appendix B in terms of the irregular eigensolutions $\{\psi_m(r)\}$ of Schroedinger's equation.

We can re-express $\omega_m(r)$ directly as a functional of $p_m(r)$ (Eq. (2.8)) as

$$\omega_m(r) = \hat{S_m}[p_m(r)] - \phi_m(r)\langle\phi_m\hat{S_m}[p_m]\rangle = \phi_m(r)\left\{\alpha_m(r) - \gamma_m\right\} - \psi_m(r)\beta_m(r) \tag{3.2}$$

where

$$\alpha_m(r) = \int_0^r dr'\psi_m(r')p_m(r') \tag{3.3}$$

$$\beta_m(r) = \int_0^r dr'\phi_m(r')p_m(r') \tag{3.4}$$

$$\gamma_m = \langle\phi_m\hat{S_m}[p_m]\rangle = \langle p_m\hat{S_m}[\phi_m]\rangle \tag{3.5}$$

and the linear operator $\hat{S_m}$, which is a pseudo inverse of the projection operator $\hat{P_m}$, is defined as in Appendix B. Inserting Eq. (3.2) into Eq. (2.6) and using the Wronskian of the regular and irreqular wavefunctions leads to

$$\Omega_m(r) = \{\alpha_m(r) - \gamma_m\}\frac{\partial}{\partial r}\left(2\phi_m(r)\frac{\partial\phi_m(r)}{\partial r}\right) - \beta_m(r)\frac{\partial}{\partial r}\left(2\psi_m(r)\frac{\partial\phi_m(r)}{\partial r}\right) \tag{3.6}$$

Now Eq. (2.5) implies that the exact OEPM exchange potential satisfies

$$\sum_m n_m\Omega_m(r=0) = 0 \tag{3.7}$$

and that by Eq. (3.6) this imposes a constraint on the 'S' (i.e. zero angular momentum) waves as

$$\sum_{m\in' S'} n_m\gamma_m\left(\frac{\partial\phi_m(r=0)}{\partial r}\right)^2 = 0 \tag{3.8}$$

An approximate V_x may not satisfies this constraint on the 'S'-waves because the values of γ_m may not be precise enough to cancel out the large contributions of the values of the derivitive of the inner orbitals at the origin. This results in a quadratic divergence in Eq. (2.14) and a breakdown in the iterative refinement of V_x.

To circumvent this difficulty an approximate regularization scheme is invoked whereby the γ_m are adjusted from their ab-initio values γ_m^0 by minimizing the Lagrangian

$$L = \frac{1}{2}\sum_{m\in' S'}(\gamma_m - \gamma_m^0)^2 + \lambda\sum_{m\in' S'}(n_m\gamma_m\dot{\phi}_m^2(0) \tag{3.9}$$

This results in a small system of linear equations to be solved for the minimially 'distance' displaced values γ_m and the Lagrange multiplier λ enforcing the constraint.

A second class of divergence, occuring in the far field, arises from the exponential decay of the denominator of Eq. (2.14). The regularization scheme we report on here simply circumvents this aspect by nulling each $\Omega_m(r)$ past the point of its outermost oscillation.

Representative results of this proceedure is illustrated in Fig. (3), which compares the 'exact' KLI error (i.e. the difference from the discretized-linear-system solution) for neutral Krypton with the results of the 'filtered' Eq. (3.6). Typically there remains a residual error in the value of the exchange potentail at the nucleus and in the vicinity of the quantal oscillations, but the bulk of the enhanced quantal oscillations is recovered.

IV. CALCULATIONAL RESULTS

Self-Consistant field calculations were performed for the ground state configuration of varying ionstages (ranging from three electrons to neutral atoms) for all elements $Z \leq 36$. The shells were populated in hydrogenic order (1s,2s,2p,3s,3p,3d,...) except for the neutrals, where the 4s shell was preferentially populated before the 3d shell to aproximate the Aufbau principle. Benchmark calculations were performed using the Hyper-Hartree-Fock program of Froese-Fischer [9], and exchange only density functional calculations were performed using the Kohn-Sham functional width Liberman's LDA code [10]. Fig. (1) shows the dramatic improvement in total energy error when using the OEPM over DF methods, and reinforces the common knowledge that DF wavefunctions should be utilized in the the HF expression of the total energy in lieu of the LDA functional. We see that the KLI approximation is not a severe degradation in the accuracy of the total energy, and that our extension of the KLI aproximation is of the order of a 20This modest improvement is not unexpected as the HF total energy functional is insensitive to functional variations of the wavefunctions.

A more relevant measure of accuracy is provided by the error in the virial relation (in the form of total plus kinetic energy). Fig. (5) shows that the KLI approximation, while still

$$E^{HHF} = \sum_i n_i T_i + \frac{1}{2}\sum_i \sum_j n_i n_j H_{ij} - \frac{1}{2}\sum_i \sum_j \sum_k c^k_{ij} X^k_{ij} \tag{A2}$$

where the independent electron contribution is

$$T_i = \int_0^\infty dr \phi_i \hat{T}_i \phi_i \equiv \int_0^\infty dr \phi_i \{-\frac{\partial^2}{\partial r^2} + \frac{L_i(L_i+1)}{r^2} - \frac{2Z}{r}\}\phi_i \tag{A3}$$

and the direct/Hartree ($H_{i,j}$) and exchange (X^k_{ij}) radial integrals are given in terms of the multipole expansion of the Coulomb interaction

$$\nu_k(r,r') = 2\frac{r^k_<}{r^{k+1}_>} \tag{A4}$$

as

$$H_{ij} = \int_0^\infty dr \int_0^\infty dr' \phi_i^2(r) \nu_0(r,r') \phi_j^2(r') \tag{A5}$$

$$X^k_{ij} = \frac{1}{2}\int_0^\infty dr \int_0^\infty dr' \phi_i(r)\phi_j(r)\nu_k(r,r')\phi_i(r')\phi_j(r') \tag{A6}$$

Note that the occupation number dependence of the exchange energy is not bi-linear

$$c^k_{ij} = \begin{cases} n_i n_j \begin{pmatrix} L_i & 0 & L_j \\ 0 & 0 & 0 \end{pmatrix}^2 & \text{if i} \neq \text{j} \\ n_i(n_i-1)\frac{4L_i+2}{4L_i+1} \begin{pmatrix} L_i & 0 & L_j \\ 0 & 0 & 0 \end{pmatrix}^2 & \text{if i=j k ¿ 0} \\ n_i(4L_i+2) \begin{pmatrix} L_i & 0 & L_j \\ 0 & 0 & 0 \end{pmatrix}^2 & \text{if i=j k=0} \end{cases} \tag{A7}$$

The variation of Eq. (A1) thus yields

$$\frac{\delta E^{HHF}}{\delta \phi_m(r')} = 2n_m\{[\hat{T_m} + V_H(r')]\phi_m(r') - h_m(r')\} \tag{A8}$$

where V_H is the Hartree potential defined in terms of the radial charge density as

$$V_H(r) = \int_0^\infty dr' \nu_0(r,r') \sum_i n_i \phi_i^2(r') \equiv \int_0^\infty dr' \nu_0(r,r') \rho(r') \tag{A9}$$

and we defined

$$h_i(r) = -\frac{1}{2n_i}\sum_j \sum_k c^k_{ij} \phi_j(r) \int_0^\infty dr' \phi_i(r') \nu_k(r,r') \phi_j(r') \tag{A10}$$

Formally we may divide h_i by ϕ_i to obtain an orbital dependant potential-like quantity, but definition would entail the introduction of spurious singularities.

significantly better than DF, is substantially degraded from OEPM results. These results reflect directly the corresponding errors in the exchange-only virial theorem derived by Levy an Perdew /citeLevy85

$$E_x = -\int d\vec{r}\rho(\vec{r})vecr \cdot \vec{\nabla}V_x(\vec{r}) \tag{4.1}$$

The virial error for our extension of the KLI approximation (Fig. (6)) does not uniformly improve results. There is a systematic trend where sodium-like through argon-like ionstages have degraded results, otherwise the improvement over KLI is roughly a factor of two, and not the order of magnitude required to approach OEPM results. In fact the error in the integral equation as measured by

$$\int dr| \int dr' K(r,r')V_x(r') - Q(r)| \tag{4.2}$$

can actually be decreased where the virial is worsened (Fig. (7)).

V. CONCLUSIONS

For configuration average total energies, where the HF expression is an insensitive functional of the wavefunctions, the KLI approximation is a rapid and superior alternative to density functional methods, and leaves little room for significant improvement vis a vis the OEPM. However more stringent measures of wavefunction quality, such a the virial theorem, leave open the desire, at least on the academic level, of constructing improved approximations to the OEPM that avoid the restrictions of that method. Iterative approaches, as outlined in this paper, despite recovering the missing quantal oscillations of the KLI approximation, falls short of this goal.

In an information theoretic sense, the (negative) of the exchange potential can be thought of as a positive definite distribution function, of which our prior state of knowledge is given by the accurate KLI approximation, which is the state of total iqnorance of the constraints imposed by the exact OEPM integral equation. Future research could try maximizing the Shannon-Jaynes entropy [12]

$$S = \int dr\{V_x(r) - V_x^{KLI}(r) - V_x(r)Log[V_x(r)/V_x^{KLI}(r)]\} \tag{5.1}$$

subject to the contraints

$$\int dr\Gamma_n(r)V_x(r) = \mu_n \tag{5.2}$$

of the moments of Eq. (1.2)

$$\Gamma_n(r) = \int dr' F_n(r')K(r',r) \tag{5.3}$$

$$\mu_n = \int dr' F_n(r')Q(r') \tag{5.4}$$

with respect to a set of linearly independent functions $F_n(r)$ in order to achieve improvements beyond the KLI approximation.

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APPENDIX A: DERIVATION OF THE OEPM INTEGRAL EQUATION

The derivation of Eq. (1.2) can be described by considering the variation of the hyper-Hartree-Fock energy with respect to orbtial variations and the the variation of orbitals with respect to a central field potential in turn.

1. Variation of hyper-Hartree-Fock

The hyper-Hartree-Fock expression for the total energy can be written in terms of reduced radial wavefunctions, normalized according to

$$\int_0^\infty dr\phi_m^2(r) = 1 \tag{A1}$$

as

2. Variation of orbitals

It is straightforward to show that the variation of eigen-orbitals ϕ_m that are solutions of

$$\{\hat{T_m} + V(r)\}\phi_m(r) = \epsilon_m \phi_m(r) \tag{A11}$$

under variation of the central field potential V(r) (with vanishing boundary conditions at the origin and infinity) is given by

$$\frac{\delta \phi_m(r')}{\delta V(r)} = -G_m(r,r')\phi_m(r) \tag{A12}$$

where

$$\hat{P_m} G_m(r,r') \equiv \{\hat{T_m} + V(r) - \epsilon_m\} G_m(r,r') = \delta(r-r') - \phi_m(r)\phi_m(r') \tag{A13}$$

A formal solution for the green's function

$$G_m(r,r') = \sum_{j \neq m}^{\infty} \frac{\phi_j(r)\phi_j(r')}{\epsilon_j - \epsilon_m} \tag{A14}$$

shows that it is real, symmetric and posseses the orthogonality property

$$\int_0^\infty dr \phi_m(r) G_m(r,r') = 0 \tag{A15}$$

3. The OEPM integral equation and Properties

By substituting Eq. (A8) and Eq. (A12) into Eq. (1.1) we are able to obtain the OEPM integral Eq. (1.2) with

$$K(r,r') = \sum_m n_m \phi_m(r) G_m(r,r') \phi_m(r') \tag{A16}$$

$$Q(r) = \sum_m n_m \phi_m(r) \int_0^\infty dr' G_m(r,r') h_m(r') \tag{A17}$$

Note that $K(r,r')$ is real symmetric, and from the orthogonality property of the greens function

thus solutions for V_x are undefined to within a constant, and the kernal itself is singular (i.e. posseses no inverse).

APPENDIX B: A COMPUTATIONAL REALIZATION OF THE GREEN'S FUNCTION

By computing a second linearly independent (irregular) solution $\psi_m(r)$ to every (regular) eigen-solution $\phi_m(r)$ of Schroedinger's equation satisfying the Wronskian

$$\phi_m(r)\frac{\partial\psi_m(r)}{\partial r} - \psi_m(r)\frac{\partial\phi_m(r)}{\partial r} = 1 \tag{B1}$$

one can show that the Green's function Eq. (A13) can be written as

$$G_m(r,r') = \phi m(r_<)\phi_m(r_>) - \phi_m(r)\Lambda_m(r') - \phi_m(r')\Lambda_m(r) + \phi_m(r)\phi_m(r')\langle\phi_m\Lambda_m\rangle \tag{B2}$$

where

$$\Lambda_m(r) = \hat{S_m}[\phi_m(r)] \tag{B3}$$

and we have defined the linear operator

$$\hat{S_m}[f(r)] = \phi_m(r)\int_0^r dr' f(r')\psi_m(r') + \psi_m(r)\int_r^\infty dr' f(r')\phi_m(r') \tag{B4}$$

which has the proprty of being a right inverse of the projection operator

$$\hat{P}_m\hat{S_m}[f(r)] = f(r) \tag{B5}$$

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FIGURES

FIG. 1. Absolute errors from HF values in the total energy for differernt ground state configurations. The configurations are ordered along the X-axis for visualization purposes by Z+(B/(Z+1)), Z being the nuclear charge and B the number of bound electrons. Red squares denote LDA total energy functional results, Blue LDA wavefunctions employed in the HF functional, Black - OEPM resulst, Green- KLI results, Yellow- the iterative extension of the KLI approximation described in the text.

FIG. 2. The exchange potential for neutral krypton in the OEPM (Red)and KLI (Blue) approximations. The dashed curves represent $r \cdot V_x \cdot 10$ to illustrate the approach to the Coulomb exchange hole tail.

FIG. 3. The difference between the exchange potential in the KLI and OEPM methods (Red) compared to the iterative correction (Blue) for singly ionized Iron in the (Closed) $3d^5 4s^1 4p^1$ excited configuration.

FIG. 4. The ratio of the total energy error from the iterative extension of the KLI approximation to that of the KLI approximation. The X-axis is as in Figure 1.

FIG. 5. The error in the virial (total plus kinetic energy). The data is presented as in Figure 1.

FIG. 6. The ratio of the errors in the virial from the iterative extension of the KLI approximation to that of the KLI approximation. The X-axis is as in Figure 1.

FIG. 7. The ratio of the errors of the integral equation, as defined by Eq. (4.2) for the iterative extension of the KLI approximation to that of the KLI approximation. The X-axis is as in Figure 1.

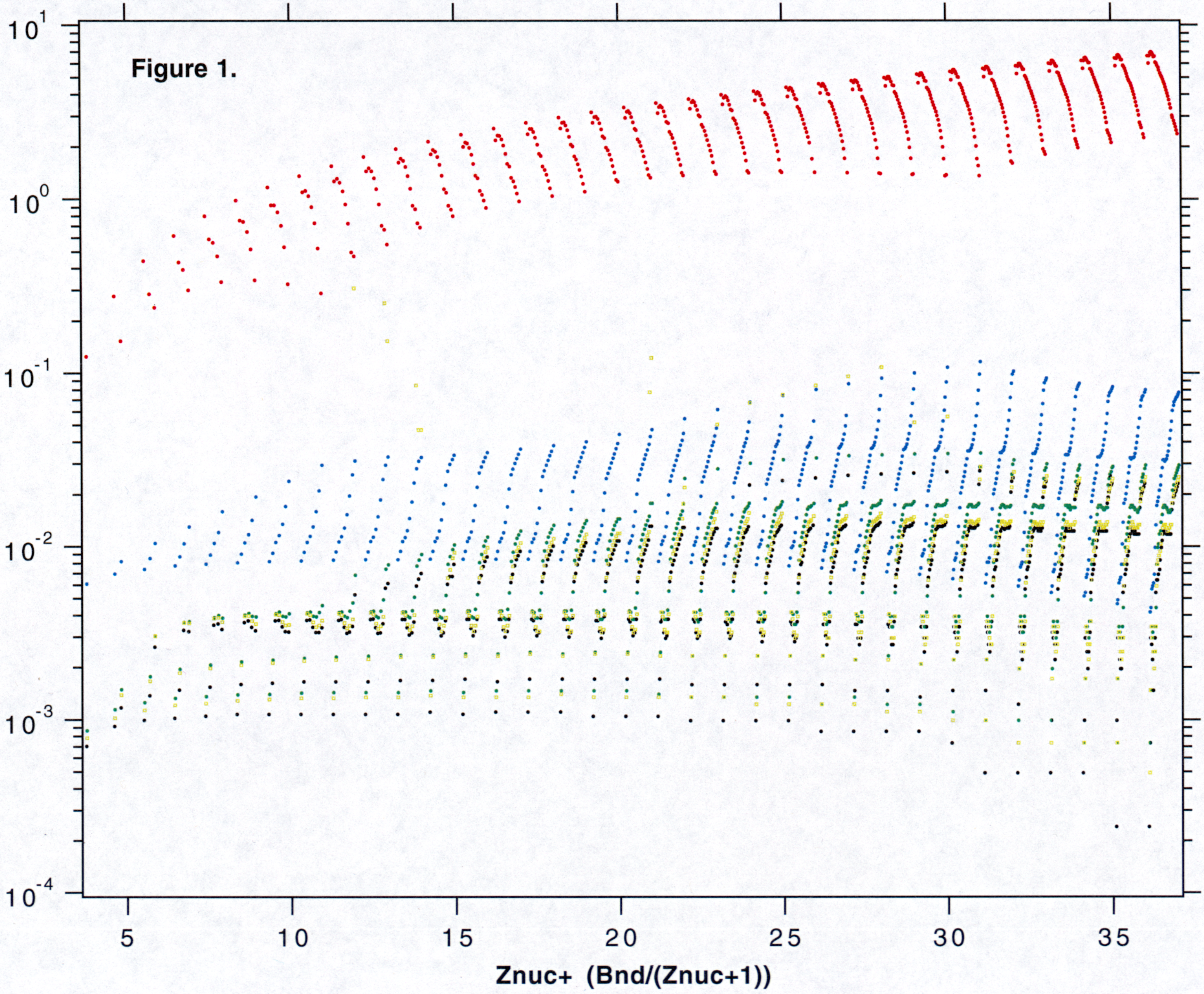


Figure 1.
10^1
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
$E_{tot}-E^{HF}_{tot}$ (Ryd)
5
10
15
20
25
30
35
Znuc+ (Bnd/(Znuc+1))

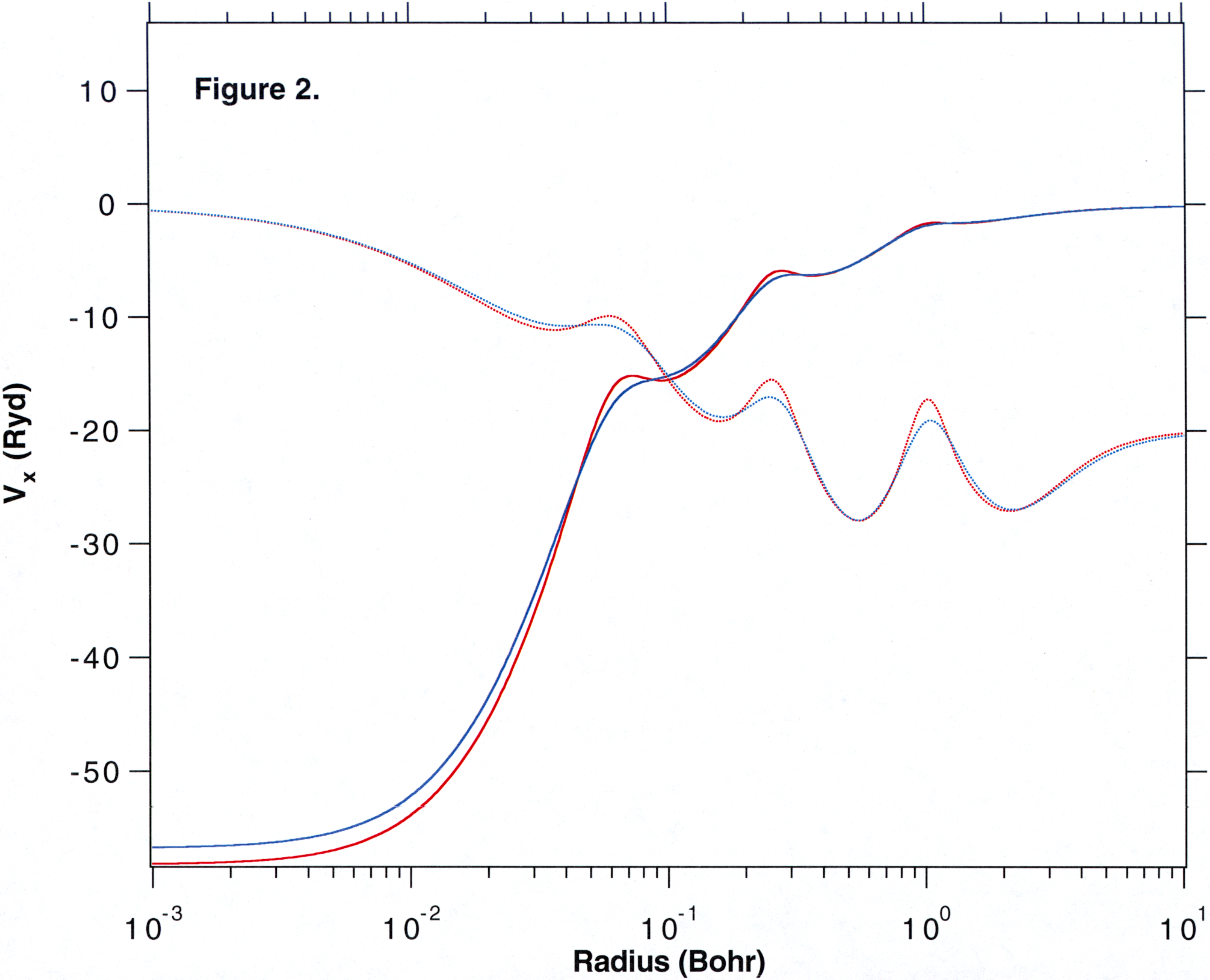
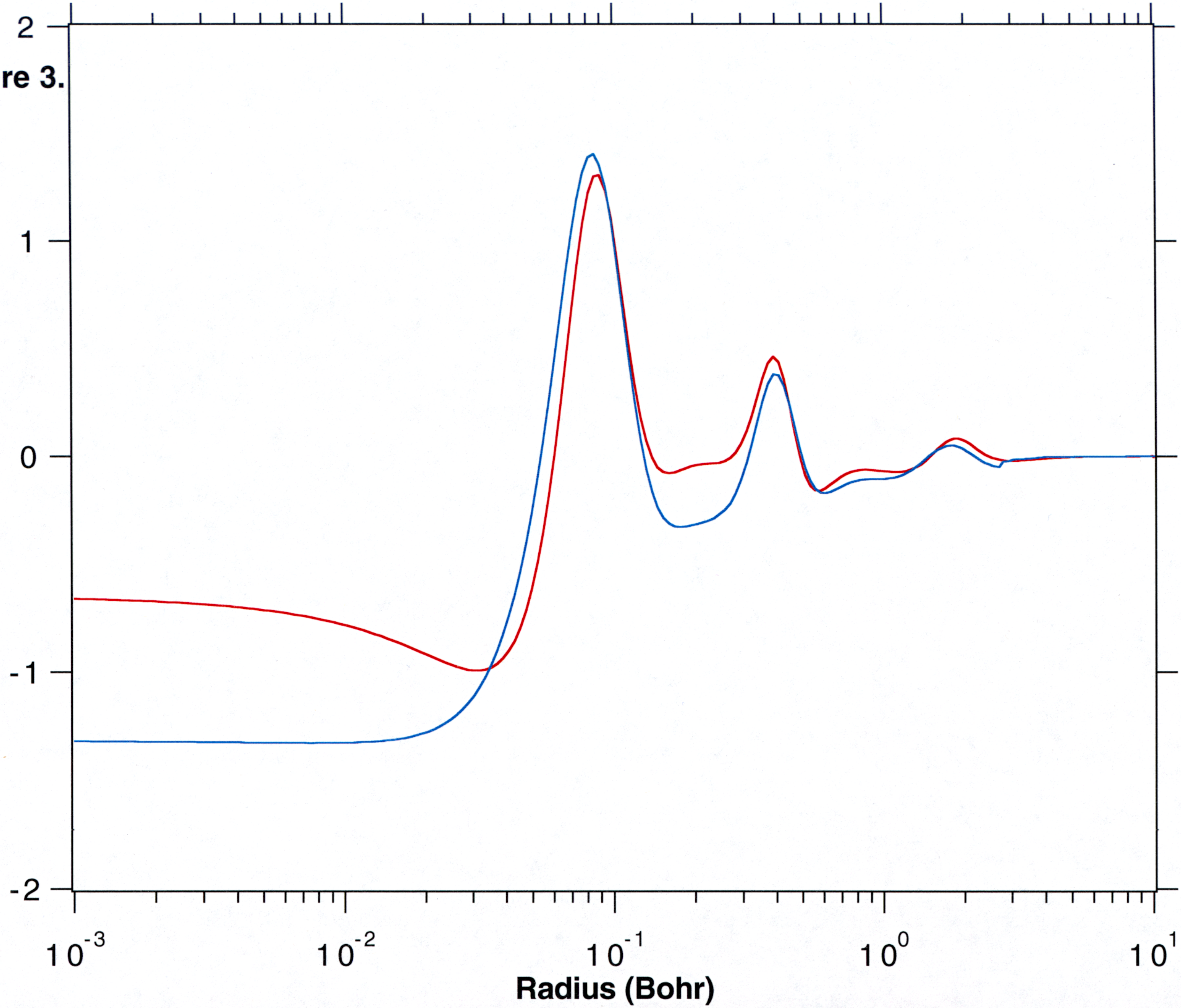


Figure 2.

Figure 3.



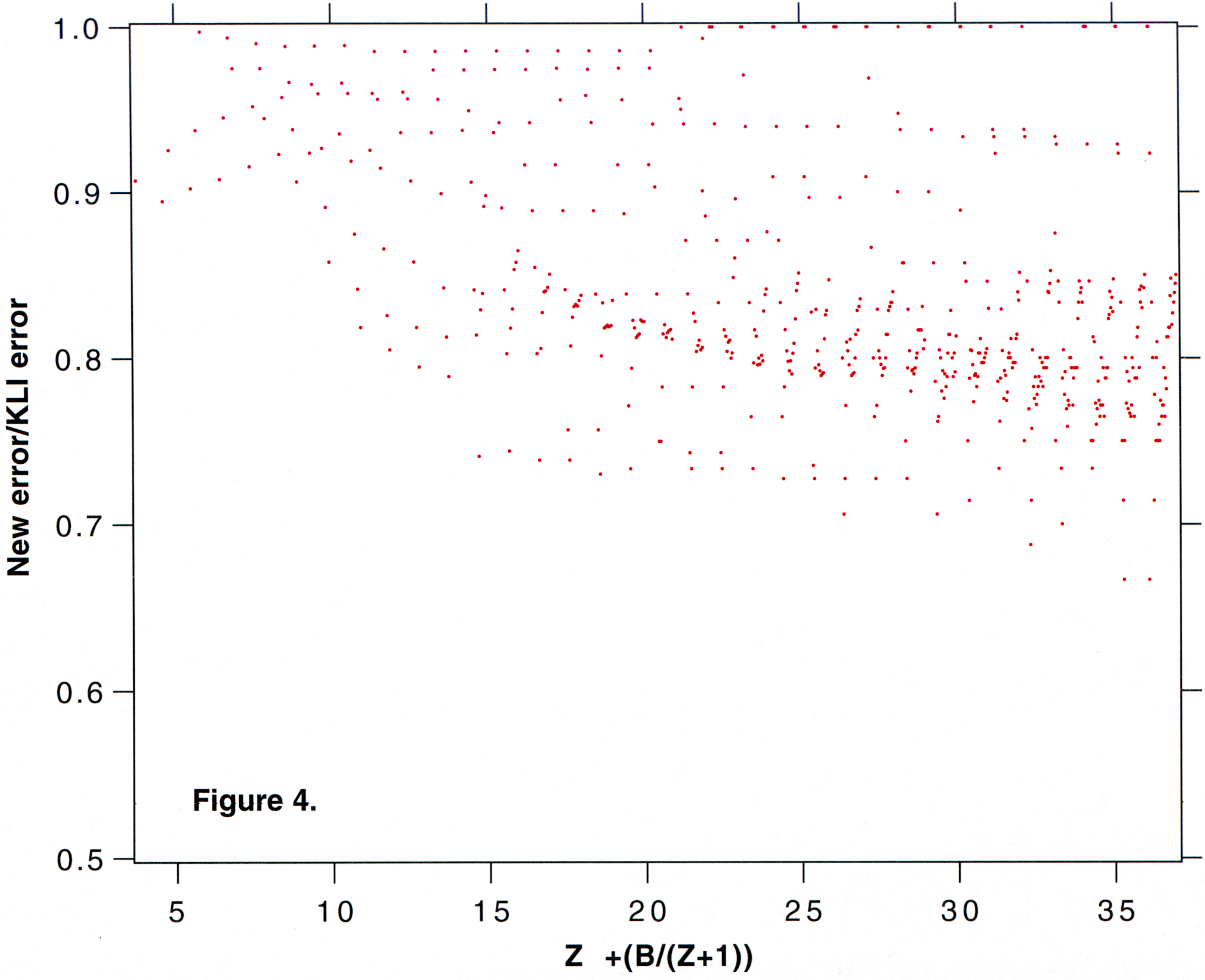
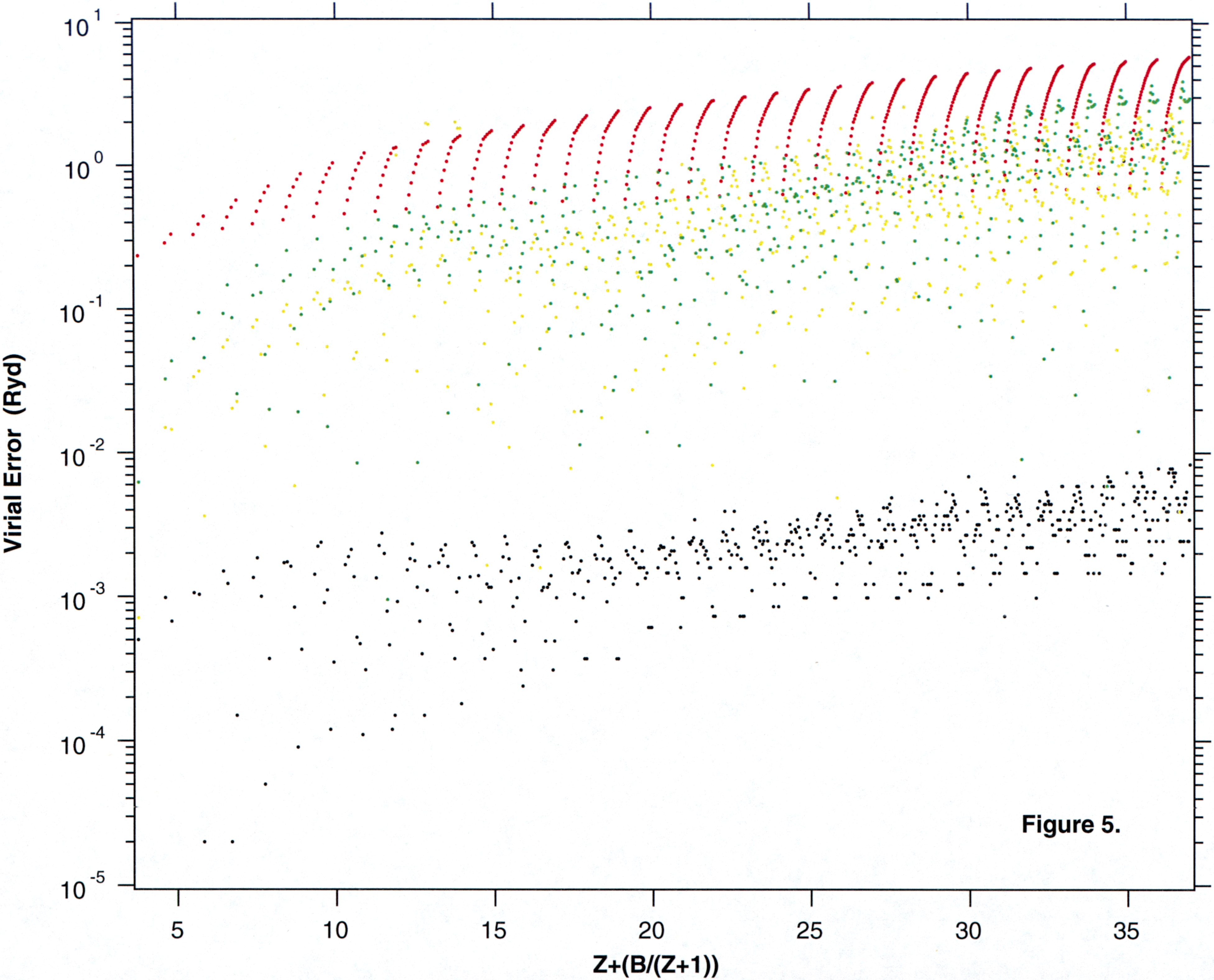


Figure 4.



Virial Error (Ryd)
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
5
10
15
20
25
30
35
Z+(B/(Z+1))

Figure 5.

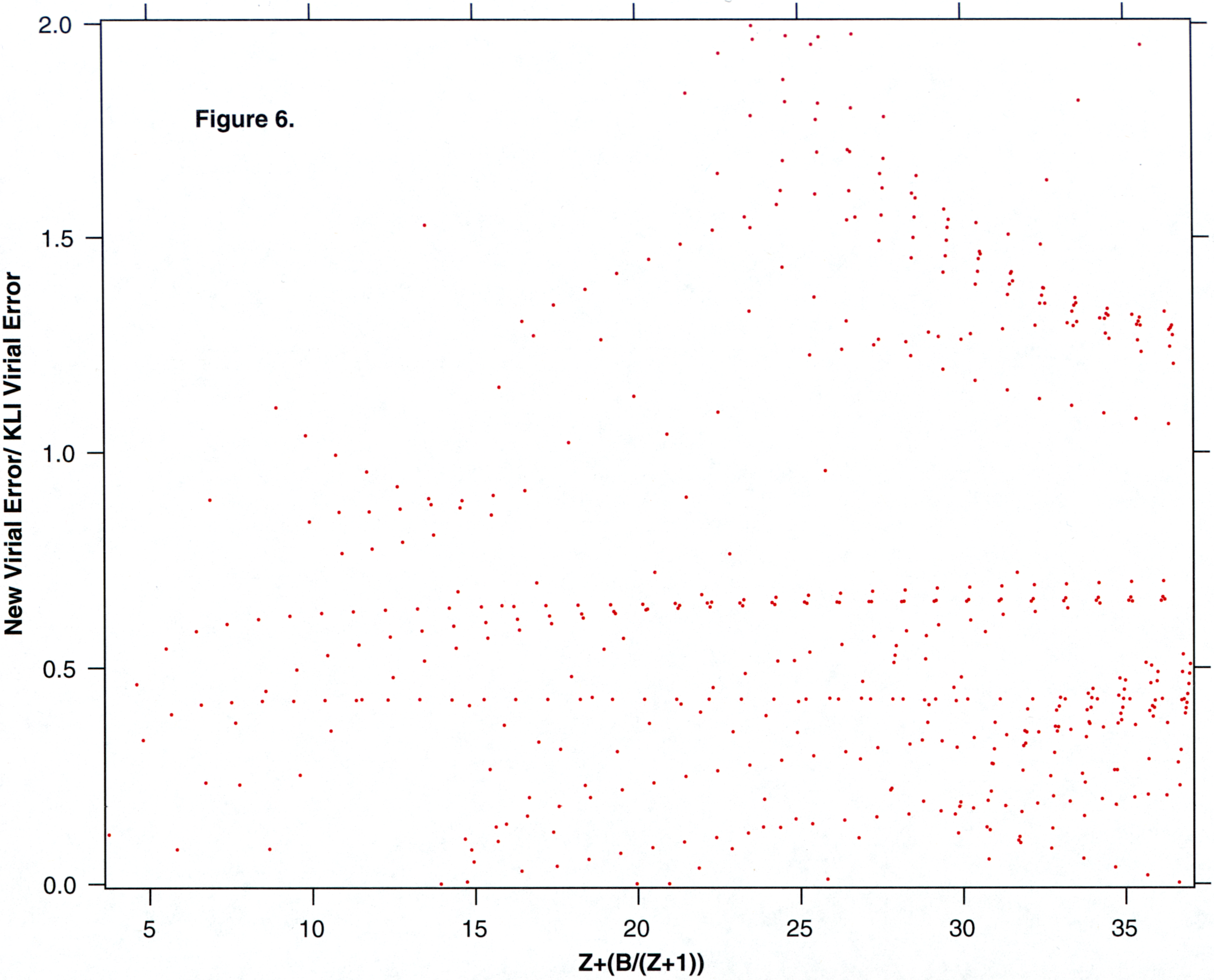


Figure 6.
New Virial Error/ KLI Virial Error
0.0
0.5
1.0
1.5
2.0
5
10
15
20
25
30
35
Z+(B/(Z+1))

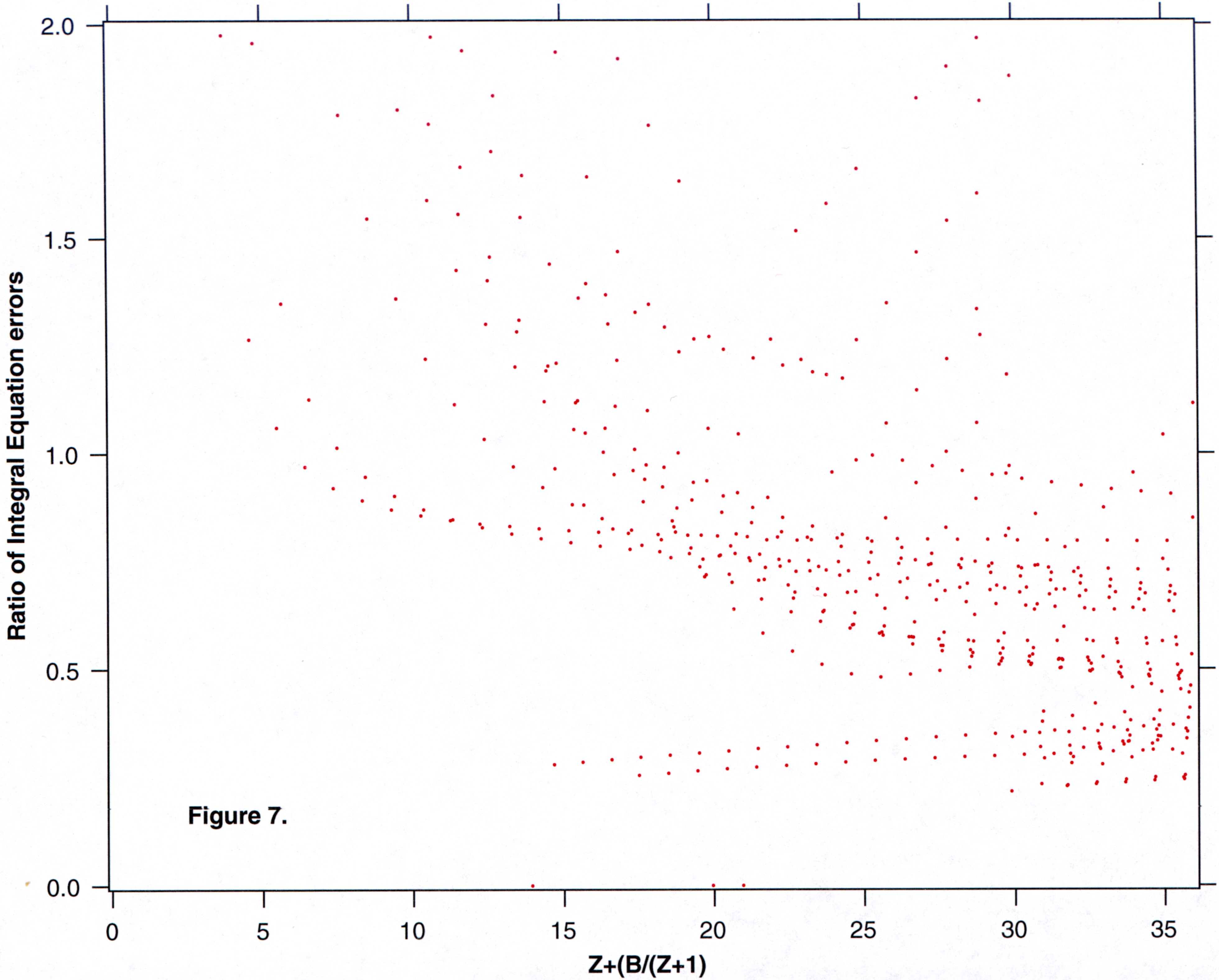

2.0
1.5
1.0
0.5
0.0
Ratio of Integral Equation errors
0
5
10
15
20
25
30
35
Z+(B/(Z+1)

Figure 7.