Dimensionality dependence of energy of heavy positive ions and the $1/Z$ expansion

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(Received 13 May 1986)

With interactions chosen to satisfy Poisson's equation in d dimensions, the form of the total energy $E(Z,N,d)$ of an atomic ion having nuclear charge Ze and N electrons is considered for large Z within the context of the $1/Z$ expansion. In particular, the form of the coefficients of this expansion is displayed at large N, the nth order coefficient being shown to be proportional to $N^{n+\alpha}$ where α is given explicitly and depends solely on dimensionality. The singular point is at $d=4$, in contrast to the situation when the $1/r$ Coulomb interaction is directly taken over into d dimensions.

I. INTRODUCTION

The work on two-electron ions by Herrick and Stillinger,[1] which has recently been developed by Herschbach,[2] is concerned with dimensional interpolation. Here we shall focus on results for heavy atomic ions with atomic number Z and N electrons, in the statistical limit, in which both N and Z tend to infinity such that $0<N/Z\leq 1$. We emphasize that there is a difference, however, in the way the appropriate Schrödinger equations are generalized to d dimensions, the definition used in Refs. 1 and 2 coinciding with that used here only for the point $d=3$. In the present work, the interactions are chosen to satisfy Poisson's equation in d dimensions.

Our starting point is that for the bare nuclear field, i.e., with no shielding allowed from the electron cloud, the ratio $E/N\mu$, with E the total energy and μ the chemical potential, has been calculated by the writer[3] as

$$\frac{E}{N\mu}=\frac{d(4-d)}{(4+2d-d^2)}=\alpha^{-1} \tag{1.1}$$

while the energy itself takes the form

$$E(Z,N,d)=F(Z,d)N^{\alpha} \tag{1.2}$$

with α given in Eq. (1.1). The function $F(Z,d)$ is exhibited explicitly in Ref. 3 for $d=1$, 2, and 3 in this model problem; it is simply $-(\frac{3}{2})^{1/3}Z^2$ for $d=3$.

We next consider the self-consistent-field problem in d dimensions. Again the writer has discussed the form of the total energy of heavy positive ions[4] for this case. Our main purpose here, especially in light of the work of Ref. 1, for the two-electron case, is to discuss the relation of the above self-consistent-field results to the $1/Z$ expansion.

II. COEFFICIENTS IN d DIMENSIONAL $1/Z$ EXPANSION IN LIMIT OF LARGE N

To introduce this, let us start from the well-known three-dimensional result that

$$E(Z,N,\,d=3)=Z^{7/3}f_3(N/Z)\,. \tag{2.1}$$

As was shown by March and White,[5] and confirmed and extended by later workers,[6,7] this result (2.1) relates to the $1/Z$ expansion

$$E(Z,N,\,d=3)=Z^2[\epsilon_{03}(N)+(1/Z)\epsilon_{13}(N)+\cdots] \tag{2.2}$$

by fixing the asymptotic behavior of the coefficients $\epsilon_{n3}(N)$ for large N as

$$\epsilon_{n3}(N)=A_{n3}N^{n+1/3}+\cdots\,, \tag{2.3}$$

where as Senatore and March[8] have recently shown

$$A_{n3}\sim\frac{A}{n^{10/3}} \tag{2.4}$$

at sufficiently large n.

We next consider the more general case of the dimensionality dependence of the corresponding coefficients $\epsilon_{nd}(N)$ of the $1/Z$ expansion

$$E(Z,N,d)=Z^{2/4-d}[\epsilon_{0d}(N)+(1/Z)\epsilon_{1d}(N)+\cdots]\,. \tag{2.5}$$

As shown in Ref. 4 in the statistical limit defined above,

$$E(Z,N,d)=Z^{(4+4d-d^2)/d(4-d)}f_d(N/Z) \tag{2.6}$$

while the first term in the generalization (2.5) of Eq. (2.2) involves the bare nuclear field problem[3] which completely determines $\epsilon_{0d}(N)$. From Eq. (1.2), this zeroth-order term varies as N^{α}, and hence the desired generalization of the $d=3$ result exhibited in Eq. (2.3) is

$$\epsilon_{nd}(N)\sim A_{nd}N^{n+\alpha}$$
$$=A_{nd}N^{[4+2d(1+2n)-d^2(1+n)]/d(4-d)}\,. \tag{2.7}$$

This asymptotic expression (2.7) is the main result of the present work. Again, as stressed in Refs. 3 and 4, $d=4$ is the singular point when interactions defined from Poisson's equation in d dimensions are employed. For the interactions adopted in Refs. 1 and 2, in contrast, there are singular points at $d=1$ and $d=\infty$.

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