Erratum: Diffusion Monte Carlo study of circular quantum dots [Phys. Rev. B 62, 8120 (2000)]

Francesco Pederiva, C. J. Umrigar, and E. Lipparini

(Received 30 May 2003; published 29 August 2003)

DOI: 10.1103/PhysRevB.68.089901 PACS number(s): 73.21.−b, 85.35.Be, 99.10.Cd

Several of the energies in Tables I and II are incorrect. Most of the errors are due to incorrect inputting of the symmetry of some of the states, others are due to incorrect converting or transcribing the energies. In particular, for $N=4$ we had a near degeneracy and a violation of Hund's first rule. The corrected result has $|L=0,S=1\rangle$ as the ground state, as predicted by Hund's rule. Hund's first rule is satisfied for all N for the confining potential used, but there is a near degeneracy for $N=10$. We present corrected versions of Tables I and II. All quantum Monte Carlo results have been recomputed with an improved Jastrow factor. All LSDA values in Table II have also been recalculated. The rms fluctuations of the local energy in VMC range from 0.008 H* for $N=2$ to 0.24 H* for the $N=13$, $|L=1,S=1/2\rangle$ state. The number of determinants, $N_{\rm det}$, in the wave functions depends on whether real or complex orbitals are employed. The values shown in Table I are for real orbitals. Not only the DMC energies, but also the VMC energies computed with LSDA and LDA orbitals agree within 1 mH* in all cases tested. All LSDA values in Table II have also been recalculated. The effective Bohr radius a_0^* should be 97.9373 Å, rather than 97.93 Å.

TABLE I. Ground state energies (in H*) and low-lying excitation energies (in mH*) for $N\leqslant 13$ dots. Also shown are the quantum numbers of the states and the number of configuration state functions $N_{\rm conf}$ and the number of determinants $N_{\rm det}$ used in constructing them. The numbers in parentheses are the statistical uncertainties in the last digit.

N	L	S	$N_{\rm conf}$	$N_{\rm det}$	E(H*), ΔE(mH*)
2	0	0	1	1	1.02164(1)
3	1	1/2	1	1	2.2339(1)
4	0	1	1	1	3.7145(1)
	2	0	1	2	41.1(1)
	0	0	1	2	66.3(1)
5	1	1/2	1	1	5.5338(1)
6	0	0	1	1	7.6001(1)
7	2	1/2	1	1	10.0342(1)
	0	1/2	1	1	27.5(1)
8	0	1	1	1	12.6900(1)
	2	1	1	1	21.9(1)
	4	0	1	2	27.5(1)
	0	0	2	3	36.0(1)
	2	0	1	2	56.1(1)
9	0	3/2	1	1	15.5801(1)
	2	1/2	2	2	28.5(1)
	4	1/2	1	2	42.6(1)
	0	1/2	2	5	55.1(1)
10	2	1	1	1	18.7232(1)
	0	0	2	3	2.9(1)
	0	1	1	1	23.3(1)
	2	0	1	2	40.0(1)
	4	0	1	2	46.7(1)
11	0	1/2	1	1	22.0738(1)
	2	1/2	1	1	15.3(1)
12	0	0	1	1	25.6356(1)
13	3	1/2	1	1	29.4938(1)
	1	1/2	1	1	39.2(1)

TABLE II. Comparison of ground state energies (in H*) for the dots with $2\leqslant N\leqslant 13$ computed by Hartree-Fock, LSDA, VMC and DMC. Also shown are the LSDA errors in the energy, $\Delta E_{\rm LSDA}=E_{\rm LSDA}-E_{\rm DMC}$, which are much smaller than the HF errors $E_{\rm HF}-E_{\rm DMC}$. The numbers in parentheses are the statistical uncertainties in the last digit.

N	$E_{\rm HF}$	$E_{\rm LSDA}$	$E_{\rm VMC}$	$E_{\rm DMC}$	$\Delta E_{\rm LSDA}$
2	1.1420	1.04684	1.02165(1)	1.02164(1)	0.02520(1)
3	2.4048	2.26308	2.2395(1)	2.2339(1)	0.0292(1)
4	3.9033	3.74632	3.7194(1)	3.7145(1)	0.0318(1)
5	5.8700	5.56919	5.5448(1)	5.5338(1)	0.0354(1)
6	8.0359	7.63500	7.6104(1)	7.6001(1)	0.0349(1)
7	10.5085	10.07176	10.0499(1)	10.0342(1)	0.0376(1)
8	13.1887	12.72691	12.7087(1)	12.6900(1)	0.0369(1)
9	16.1544	15.61889	15.5996(1)	15.5801(1)	0.0388(1)
10	19.4243	18.76357	18.7496(1)	18.7232(1)	0.0404(1)
11	22.8733	22.11130	22.1018(1)	22.0738(1)	0.0375(1)
12	26.5490	25.67597	25.6659(1)	25.6356(1)	0.0404(1)
13	30.4648	29.53617	29.5295(1)	29.4938(1)	0.0424(1)

