# Supplementary Material for "Correlation Induced Inhomogeneity in Circular Quantum Dots"

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In this supplementary material we present a comparison of the energies we obtain with those obtained previously by two other methods. The three cases compared are (a) our results using the diffusion Monte Carlo (DMC) method, (b) the path integral Monte Carlo (PIMC) results of Egger, et al. (Ref. 15 of the paper),[1] and (c) the full configuration interaction (CI) results of Rontani, et al. (Ref. 14 of the paper).[2] In order to make the comparison, we use values for the electron number and interaction strength for which results have been published in Refs 1 and 2. Both of those references use $\lambda = 1/\sqrt{\omega}$ (in atomic units) to characterize the interaction strength. We will compare the ground state energies obtained for $N = 3$, 6 and 8 and $\lambda =$ 2-10. We will demonstrate that the DMC method yields a much more accurate and *lower* energy, particularly for strong interactions, than either other method.

The comparison is made in the Table. As all three methods rely on the energy minimization principle, the method that finds the lowest energy gives the best result. As mentioned in the main text, it is known that the DMC energy is an upper bound on the true ground state energy. Note the following points in the Table:

1. Since the DMC and CI calculations fix both total $L$ and total $S$, they can be compared directly – energies for several $(L, S)$ cases are given. The PIMC calculation fixes only $S_z$, thus mixing states of all $L$ and $S$ which satisfy this constraint. Because of this difference, the PIMC results are presented separately, to the right of the others.
2. For small $\lambda$, the DMC results match those from PIMC and CI. Note the large difference in the size of the statistical error between our results and those of Ref 1 – the DMC statistical error bars are 100 to 1000 times smaller than those of PIMC. In the case $N = 3$, $\lambda = 4$, for instance, the PIMC statistical error bar is larger than the energy difference of the two spin states. In the case, $N = 8$, $\lambda = 2$, the $S_z = 1$ PIMC energy is about one standard deviation lower than our $(0, 1)$ result.
3. For $N = 3$, $\lambda = 10$ and $S = 3/2$ the CI energy is the lowest, demonstrating that for a small system exact diagonalization can be carried out very effectively. We could obtain a lower DMC energy by using more than one determinant for this state.
4. At large $\lambda$ and $N = 6$ or 8, the DMC energies are smaller than either PIMC and CI. For instance, for $N = 8$ and $\lambda = 8$, the energy of Ref 1 is about $4\sigma$ higher than our energy, and the difference in energy that we find between the $S = 1$ and $S = 2$ states is far smaller than the statistical error bar of Ref 1. The fact that the CI energies for $N = 6$ are substantially higher than ours suggests that those calculations are not converged (the results of Ref 2 for $N = 8$ are omitted from the Table because they state their calculations are not converged in that case).
5. The case $N = 6$, $\lambda = 8$, $S = 1$ deserves special mention. Since the $(0, 2)$ state is lower than any of the $S = 1$ states, a calculation which fixes only $S_z$ will pick it out, missing the $S = 1$ states entirely. Thus we have listed the PIMC $S_z = 1$ calculation in the same row as our $(0, 2)$ value rather than the $(1, 1)$ value.

6. The ground state spin and angular momentum is an important outcome of an energy study such as the three compared here. In particular, one would like to know whether Hund's rules are satisfied – both the first (maximum $S$ consistent with shell structure) and second (minimum $L$ consistent with the first rule). For $N = 3$ and large $\lambda$, all three calculations show that Hund's first rule is violated ($S = 3/2$ is the ground state). For larger $N$, we disagree rather strikingly with Ref 1: *we find no violations of Hund's first rule for any other case in our entire parameter range.* Because this conclusion is based on energies which are all lower than those of Ref 1, we believe it is correct. We do, however, find numerous examples of violations of Hund's second rule, a topic inaccessible to the PIMC method of Ref 1 since $L$ is not fixed. For example, in the $N=8$, $\lambda=8$ case, the ground state is $(2, 1)$ rather than $(0, 1)$.

All three methods compared here do, of course, involve approximations and errors; before closing, we comment briefly on these in the three cases:

- For our DMC method, the main error of concern is that caused by the fixed-node approximation coming from our use of a particular trial wavefunction. This error is difficult to quantify. We have investigated it by increasing the number of Slater determinants used in the trial wavefunction (see Methods section of paper). An estimate of this fixed-node error yields a value of twice (for $\lambda = 3.45$) or four times (for $\lambda = 10$) our statistical errors, suggesting that the fixed-node error is under control in these cases.
- In the CI calculations, the many-body basis set must be truncated at some point, and so the main error is simply convergence with regard to the size of the basis set used. As the size of the Hilbert space grows very rapidly with $N$, this generally restricts these calculations to small $N$. Ref 2 comments that they were unable to get converged results for $N = 8$; hence, we have omitted these energies from the Table. In fact, the comparison with the DMC results for $N=6$ shows that even in that case, the CI results are not converged.
- For the PIMC calculations of Ref 1, there are three main problems. First, the method does not respect the space-rotational and spin-rotational symmetry of the Hamiltonian; thus, only $S_z$ is fixed – $L$ and $S$ cannot be directly determined. Second, the calculation is done at non-zero temperature. This becomes particularly a problem for strong interaction where many spin states have a similar energy. Third, the statistical error in the method is quite large.

In conclusion, in this Supplementary Material we have compared the energies obtained by three different computational methods. We find that the DMC method produces the best energies over almost the whole parameter range of comparison.

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[1] Egger, R., Häusler, W., Mak, C. H. & Grabert, H. Crossover from Fermi liquid to Wigner molecule behavior in quantum dots. Phys. Rev. Lett. **8**2, 3320 (1999); **8**3, 462(E) (1999).

[2] Rontani, M., Cavazzoni, C., Bellucci, D., and Goldoni, G. Full configuration interaction approach to the few-electron problem in artificial atoms. Preprint, cond-mat/0508111 (2005).

Table I: The ground state energy of a circular 2D quantum dot obtained by three different computational methods – diffusion quantum Monte Carlo (DMC), full configuration interaction (CI), and path-integral quantum Monte Carlo (PIMC). $N$, $L$, and $S$ specify the number of electrons in the dot, their angular momentum, and their spin. The energy is given in units of $\hbar\omega$, the characteristic energy of the external parabolic confining potential. $\lambda = 1/\sqrt{\omega}$ (in atomic units) characterizes the strength of the interactions.

| $N$ | $\lambda$ | $r_s$ (approx) | $L$ | $S$ | DMC: this work | CI: Ref 2 | $S_z$ | PIMC: Ref 1 |
|---|---|---|---|---|---|---|---|---|
| 3 | 4 | 5.7 | 1 | 1/2 | 11.0408(5) | 11.043 | 1/2 | 11.05(1) |
| | | | 0 | 3/2 | 11.05243(4) | 11.053 | 3/2 | 11.05(2) |
| | 6 | 9.1 | 1 | 1/2 | 13.4672(7) | 13.467 | | |
| | | | 0 | 3/2 | 13.43856(8) | 13.438 | 3/2 | 13.43(1) |
| | 10 | 16.0 | 1 | 1/2 | 17.6286(6) | 17.630 | | |
| | | | 0 | 3/2 | 17.5905(1) | 17.588 | 3/2 | 17.60(1) |
| 6 | 8 | 12.5 | 0 | 0 | 60.3251(3) | 60.64 | | |
| | | | 1 | 1 | 60.4027(3) | 60.71 | | |
| | | | 0 | 2 | 60.3520(2) | 60.73 | 1 | 60.37(2) |
| | | | 0 | 3 | 60.3924(2) | 60.80 | 3 | 60.42(2) |
| | 10 | 16.3 | 0 | 0 | 68.9202(5) | 69.74 | | |
| | | | 1 | 1 | 69.0568(7) | | | |
| | | | 0 | 2 | 68.9254(6) | 69.81 | | |
| | | | 0 | 3 | 68.9458(4) | 69.86 | | |
| 8 | 2 | 2.1 | 0 | 0 | 46.8070(4) | | | |
| | | | 2 | 0 | 46.8746(4) | | | |
| | | | 4 | 0 | 46.7793(3) | | | |
| | | | 0 | 1 | 46.6787(3) | | 1 | 46.5(2) |
| | | | 2 | 1 | 46.7560(4) | | | |
| | | | 1 | 2 | 46.9170(4) | | 2 | 46.9(3) |
| | | | 0 | 2 | 47.4058(4) | | | |
| | | | 3 | 3 | 47.4035(3) | | 3 | 47.4(3) |
| | | | 0 | 4 | 48.1810(4) | | 4 | 48.3(2) |
| | 8 | 12.2 | 0 | 0 | 102.9402(4) | | | |
| | | | 2 | 0 | 102.9464(4) | | | |
| | | | 4 | 0 | 103.0465(4) | | | |
| | | | 0 | 1 | 102.9263(4) | | | |
| | | | 2 | 1 | 102.9198(4) | | | |
| | | | 1 | 2 | 102.9280(4) | | 2 | 103.08(4) |
| | | | 0 | 2 | 103.1965(4) | | | |
| | | | 3 | 3 | 103.0185(3) | | 3 | 103.19(4) |
| | | | 0 | 4 | 103.0464(4) | | 4 | 103.26(5) |