Crossover from Fermi liquid to Wigner molecule behaviour in parabolic quantum dots

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Quantum dots as finite many-particle systems are interesting and well suited to study correlation effects. Parameters, like the particle number or the charge density can be tuned within wide ranges. Direct experimental access to the discrete levels makes a detailed understanding of the many-particle features amenable [1,2]. Weak interactions can be incorporated into effective single-particle orbitals, e.g. within the mean-field approximation. This is no more possible for strong interactions or, equivalently, low carrier densities where a crossover into the Wigner regime arises with spatial instead of orbital shell structure [3]. Here we quantify this crossover together with the amount of correlations by comparing with mean-field results.

Quantum Monte Carlo (QMC) simulations can provide reliable data, once the infamous sign problem is circumvented. We adopt the recently developed multilevel blocking algorithm [4] to quantum dots in order to tackle the sign problem. Exact diagonalisation results and QMC data are compared with results of an unrestricted Hartree–Fock (HF) calculation.

We investigate a parabolic quantum dot at zero magnetic field

$$H = \sum_{j=1}^{N} \left(\frac{\boldsymbol{p}_j^2}{2m^*} + \frac{m^*\omega_0^2}{2}\boldsymbol{x}_j^2 \right) + \sum_{i<j=1}^{N} \frac{e^2/\kappa}{|\boldsymbol{x}_i - \boldsymbol{x}_j|},$$

where the positions (momenta) of the electrons are denoted by $\boldsymbol{x}_j(\boldsymbol{p}_j)$. The effective mass is m^*, and the dielectric constant is κ. The length scale $l_0 = \sqrt{\hbar/m^*\omega_0}$ from the confinement defines the parameter $\lambda = l_0/a_B$ measuring the interaction strength, with the effective Bohr radius a_B.

QMC and HF calculations have been carried out for different z-components $S_z = (N_\uparrow - N_\downarrow)/2$ of the total spin. The QMC simulation is done for very low temperature $T = 0.1\hbar\omega_0/k_B$. Data for the ground state energy are given in Table 1 and compared with results of HF calculations. For $N = 2$ we compare the HF results with exact diagonalisation (both $T = 0$).

We notice that for the polarised states the HF energies are only about 1–2% higher than the exact energies throughout the whole range of the coupling constants λ. For dots with lower spin S_z the error is larger, about 12–24% in the case of the singlet $N = 2$ and about 7% in the case of $N = 4$, $S_z = 1$. As is well known, these discrepancies arise from the HF exchange potential, which incorrectly favours the filling of parallel spins, and therefore leads to un-physically high spin for the ground state.

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Table 1
Results of exact diagonalisation and QMC versus HF for the energy for various $\{N,S,\lambda\}$ parameter sets. Bracketed numbers denote statistical errors of QMC

N	S_z	λ	$E_0^{\text{exact}}/\hbar\omega_0$	$E_0^{\text{HF}}/\hbar\omega_0$
2	1	2	4.142	4.168
2	0	2	3.721	4.185
2	1	4	5.119	5.189
2	0	4	4.848	5.878
2	1	6	5.990	6.096
2	0	6	5.784	7.117
2	1	8	6.787	6.919
2	0	8	6.618	8.177
2	1	10	7.528	7.679
2	0	10	7.384	9.138
N	S_z	λ	$E_0^{\text{QMC}}/\hbar\omega_0$	$E_0^{\text{HF}}/\hbar\omega_0$
4	2	2	14.30(5)	14.346
4	1	2	13.78(6)	14.295
4	2	4	19.42(1)	19.578
4	1	4	19.15(4)	20.265
4	2	6	23.790(12)	24.109
4	1	6	23.62(2)	25.205
4	2	8	27.823(11)	28.172
4	1	8	27.72(1)	29.618
4	2	10	31.538(12)	31.908
4	1	10	31.48(2)	33.684
7	7/2	8	80.59(4)	81.631
7	5/2	8	80.45(4)	82.501

We emphasise the importance of breaking the rotational symmetry, which lowers the energies most efficiently for the polarised states at higher interaction strength λ. This can also be seen in the HF one-particle densities which exhibit the classical behaviour of localised electrons in geometric shells, whereas the exact and QMC densities are spherically symmetric and the spatial shell structure can only be revealed by the two-particle correlation function [3]. HF calculations with rotational symmetry [5] lead to larger deviations for strong correlation $\lambda \gg 1$, and unrestricted HF is essential to find the crossover to a Wigner molecule as seen previously in the QMC study [3].

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