Isotropic quantum dots at strong interactions Wolfgang Häusler*

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Recent experimental progress allows detailed measurement of excited levels of small quantum dots by nonlinear transport [1]. A parabolic confining potential

$$H = \sum_{i=1}^{N} \frac{\mathbf{p}_{i}^{2}}{2m^{*}} + \frac{m^{*}\omega_{0}^{2}}{2} \sum_{i=1}^{N} \mathbf{x}_{i}^{2} + \sum_{i < j} \frac{e^{2}/\kappa}{|\mathbf{x}_{i} - \mathbf{x}_{j}|}$$
(1)

is regarded as most realistic [2]. The effective mass m^* and the dielectric constant κ are material parameters, and \mathbf{x}_j (\mathbf{p}_j) are electron positions (momenta) in two dimensions. All of the eigenstates of H are simultaneously eigenstates to \hat{S}^2 , with eigenvalues S(S + 1).

In the limit of strong interactions or, equivalently, low particle densities, where the electrons form a Wigner molecule (WM) [3], the pocket state method (PSM) has been used to determine the energy spectra [4]. Up to now this method was restricted to quantum dots of low symmetries, like polygons [5]. Here, we extend this method to allow for azimuthally symmetric quantum dots and compare the results with those obtained by exact quantum Monte Carlo (QMC) [3].

It seems tempting to separate out the conserved overall rotations associated with total angular momentum ℓ . However, the remaining normal coordinates then would no more represent identical quantum particles obeying Pauli's principle but linear combinations of such particles. Within the PSM it is crucial to know the result of particle permutations in order to assign the correct total

spins *S* to the eigenstates by group theoretical arguments [4].

Therefore, we treat all of the possible particle exchanges on an equal footing, including rotations if they correspond to permutations. Depending on the geometry of the WM, rotations by $2\pi/p$ with p > 1 leave the electron places invariant so that the Pauli principle relates ℓ with S. Up to $N \leq 8$ the WM in (1) is known [3] to be quite symmetric: the electrons form one spatial shell $(N \leq 5)$ so that p = N, or one central electron occupies the center (i.e. p = N - 1).

It is crucial for the pocket state approximation that lowest spin sensitive excitations are smaller in energy than charge (plasmon) excitations. In the cases of unsymmetric quantum dots this is fulfilled due to their exponential decay $\sim \exp - \sqrt{r_s}$ with reducing density – plasmons decrease only according to a power law $\sim r_s^{-3/2}$ for Coulomb repulsions. With their slightly faster decay $1/2I \sim r_s^{-2}$ the rotational excitations justify the PSM.

Entries of the pocket state matrix $t_{\rm R} = p^2/8\pi^2 I$ associated with rotations by $2\pi/p$ ensure lowest rotational excitation energies $\sim \ell^2/2I$ (the momentum of inertia *I* follows from the radial charge density distribution). We measure the interaction strength by $y = 1/(1 + t/t_{\rm R})$ with *t* being the nearest-neighbour integral (which exponentially dominates over any of the higher-order exchanges, apart from zero modes). The limit $y \rightarrow 1$ corresponds to a rigid WM and strong interactions. In this limit, the PSM becomes exact. The lower bound for possible values for *y* can be estimated as $y > 1/(1 + (\pi^2/4)p)$ since 2*t* cannot exceed the Fermi energy in the non-interacting limit.

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Fig. 1. Low-energy levels using pocket states versus y for N = 3 in units of t_{R} .

For weak interactions the ground state for N = 3 (cf. Fig. 1) is unpolarized, $S = \frac{1}{2}$. A transition into the spin polarized ground state $S = \frac{3}{2}$ is found above a critical interaction strength. Assuming Coulomb interactions we estimate this transition to occur when $\omega_0 < 0.5$ meV. This spin polarization is an exact consequence of the correlations and not the result of a mean field approximation or of a magnetic field. It should show up as a 'spin blockade' [6], even in linear transport for transitions between the N = 2 and N = 3 ground states. This result has also been obtained in QMC calculations [3].

For N = 4 (not shown) we confirm that the Hund's rule result S = 1 stays ground state for all interaction strengths [3]. Fig. 2 shows the low-energy levels for N = 5, that were not obtained previously. The ground state remains unpolarized $S = \frac{1}{2}$ up to strong interactions, though its character changes. The polarized state, however, approaches the ground state and can therefore cause negative differential conductances in the non-linear transport [6] at sufficiently small confinement energies.

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Fig. 2. Low-energy levels using pocket states versus y for N = 5 in units of $t_{\rm R}$.

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