Violation of non-interacting v-representability of the exact solutions of the Schrödinger equation for a parabolic two-electron quantum dot in a homogeneous magnetic field

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In density functional theory it can be shown that the electron density of the ground state (GS) can be calculated from a model system of non-interacting particles in a properly chosen external potential, the Kohn-Sham (KS) system. This property is called non-interacting v-representability (NIVR). It follows from the fact that all mutual mappings between the external potential, many body wave function (WF) and electron density of the GS are invertible [1].

In the basic work on (non-relativistic) current density functional theory (CDFT) [2] NIVR of both densities (charge- and the paramagnetic current density) has been tacitly assumed, because the invertibility of the mapping of the external potentials (scalar- and vector potential) on the wave function has never been proven. In the contrary, in [3] has been shown, that different external potentials can provide the same WF. This rules the invertibility of the above mentioned mapping out, but does not say anything about NIVR.

We have shown by means of the exact solutions for the two-electron system in a parabolic confinement and a homogeneous magnetic field [4] that the exact densities are not always NIVR, or equivalently, that an exact KS system does not always exist. Whether it exists depends on the total angular momentum of the GS. (It is well known that the modulus of the orbital angular momentum L of the GS grows step-wise with increasing magnetic field connected with singlet-triplet oscillations.)

If the GS is a singulet (L is even) both densities are NIVR if the vorticity of the exact solutions vanishes. For L=0 this is trivially guaranteed because the paramagnetic current density vanishes in this state. (The gauge invariant mechanical current density does not vanish, though.) Fig.1 shows, that the vorticity based on the exact solutions for the higher L does not vanish, in particuler for small r.

If the GS is a triplet (L is odd) we can show, that there is no circular symmetric KS system which can provide the exact densities, except for L= – 1. Therefore, in this case NIVR cannot be ruled out in general, but it has been shown that common practise in self-consistent CDFT computations, where NIVR with a circular symmetcc KS system is assumed on the basis of the circular symmetry of the real system, is not rigorously justified. However, this does not mean, that all these results are completely wrong.

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Figure 1: Vorticity for exact singlet states for effective confinement frequency (see [4]) =1 and total orbital angular momenta L= – 2 and L= – 4.