Asymptotic behaviour of exchange-correlation potentials from the linear-response Sham-Schlüter equation

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The linear-response Sham-Schlüter equation can be used to calculate an exchange-correlation potential starting from a given approximation for the self-energy. The asymptotic behaviour of these potentials is however much debated, some recent works suggesting that they could blow up in finite systems. Here we investigate the asymptotic behaviour of the linear-response Sham-Schlüter potentials in the GW and second order approximations for the self-energy. We show that these potentials have the expected $-1/r$ behaviour in finite systems (due to exchange), and that the correlation potential itself has a $-\alpha/(2r^4)$ tail (where $\alpha$ depends on the self-energy). We also provide further justification for the quasiparticle approximation to the linear-response Sham-Schlüter equation, that is much simpler to solve while being likely of comparable accuracy. Calculations for real molecules or solids using this approximation should be within the reach of present computers.