Interaction effects in the thermodynamic properties of quantum dots: a Hartree-Fock study.

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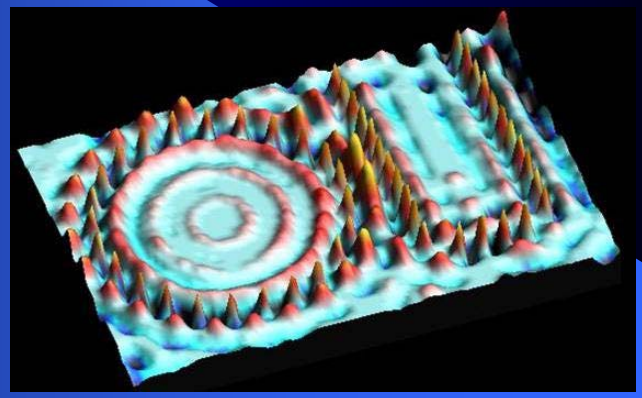
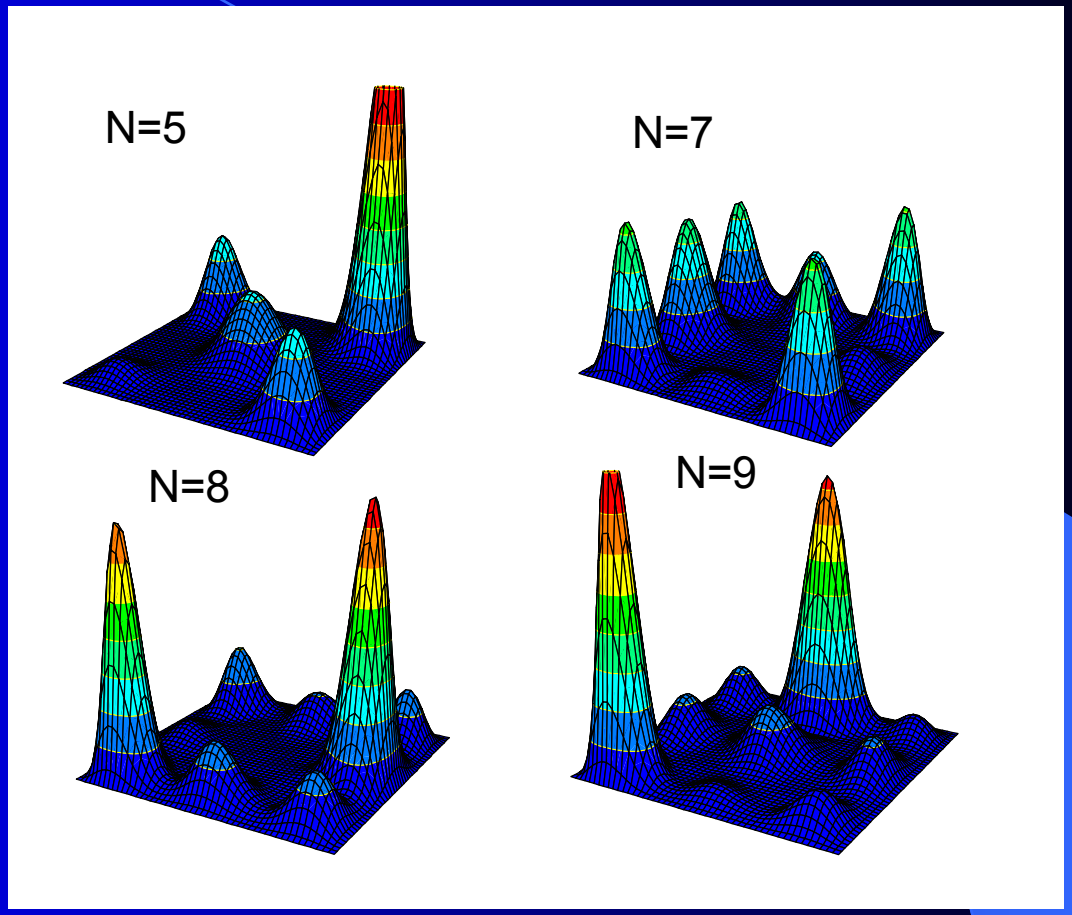
Support:



System of N interacting e^-

- N=10-20 interacting electrons confined in a Square QD.
- Orthogonal magnetic field B.
- Hartree-Fock at $T \neq 0$.



$$H = \sum_{i=1}^{N} \frac{1}{2m^*} \left(\mathbf{p}_i + \frac{e}{c} \mathbf{A}(\mathbf{r}_i) \right)^2 + u_{Square}(\mathbf{r}_i) + \sum_{i.j=1}^{N} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}$$

Self-Consistent Hartree-Fock at $T \neq 0$

$$h_0 = \frac{1}{2m^*}\left(\mathbf{p} + \frac{e}{c}\mathbf{A}(\mathbf{r})\right)^2 + u_{SQUARE}(\mathbf{r})$$

$$n_i = \left\{\exp\left[\left(\varepsilon_i^{HF} - \mu\right)/k_B T\right] + 1\right\}^{-1}$$

$$h_0(\mathrm{r})\phi_i(\mathrm{r}) + \sum_j \left[n_j \int d\mathbf{r}' \phi_j^*(\mathrm{r}') v(\mathrm{r},\mathrm{r}') \phi_j(\mathrm{r}') \right] \phi_i(\mathrm{r})$$

$$-\sum_j \left[n_j \int d\mathbf{r}' \phi_j^*(\mathrm{r}') v(\mathrm{r},\mathrm{r}') \phi_j(\mathrm{r}) \phi_i(\mathrm{r}') \right] = \varepsilon_i^{HF} \phi_i(\mathrm{r})$$

Self-Consistency; GS Energy

$$E^{HF} = \frac{1}{2}\sum_i n_i \left(\varepsilon_i^{HF} + \langle \phi_i | h_0 | \phi_i \rangle\right)$$

Interaction strength

$$r_s = \frac{L}{a_B^* \sqrt{\pi N}}$$

Contributions to E^{HF}

$$E_g^{HF} = \sum_{i=1}^{N} n_i \langle \phi_i | h_0 | \phi_i \rangle +$$

$$+ \frac{1}{2} \sum_{i,j} n_i n_j \left(\langle \phi_i \phi_j | v | \phi_i \phi_j \rangle - \langle \phi_i \phi_j | v | \phi_j \phi_i \rangle \right)$$

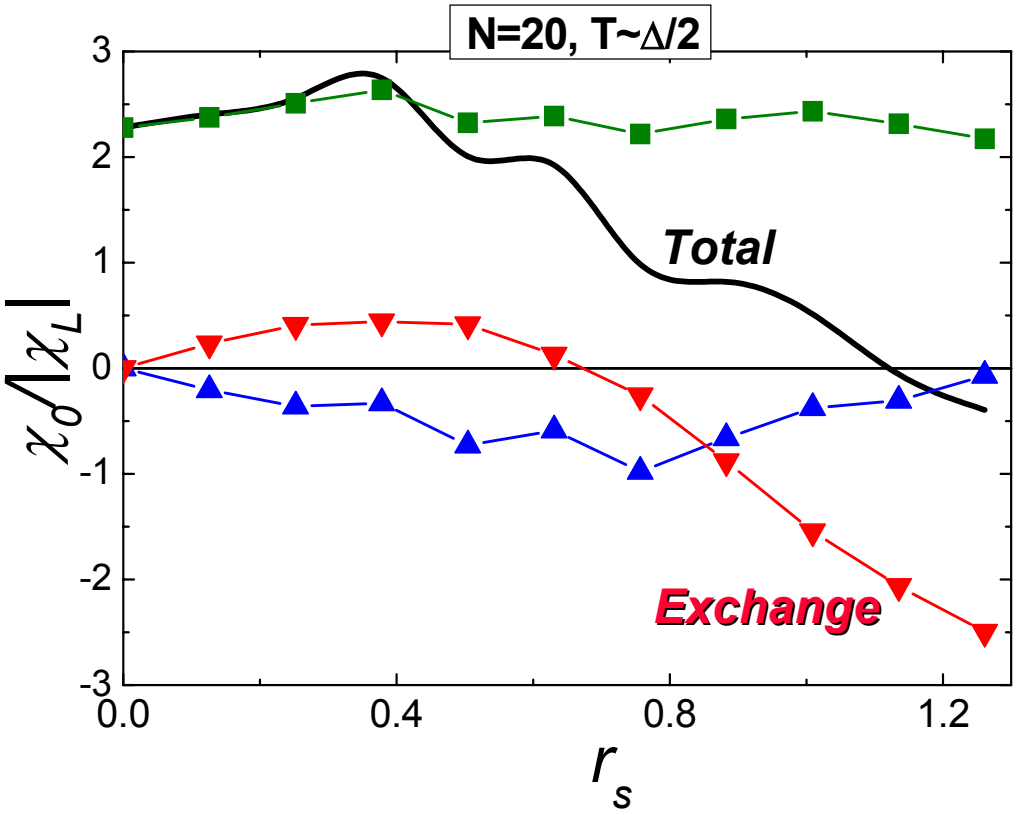
$$E_g^{HF} = E_{KINETIC} + E_{DIRECT} + E_{EXCHANGE}$$

Typical Parameters:

- N~10 – 20 (some runs with up to 40 electrons).
- r_s ~ 1 – 3 (weakly to morerate interacting regime).
- T ~ Δ – 3Δ ($\Delta \rightarrow$ mean level spacing)

Magnetic Susceptibility
Exchange contribution

Exchange is the largest contribution for $r_s \sim 1$



$$\chi(B) = -\frac{1}{L^2}\frac{\partial^2 F}{\partial B^2}$$

$$\chi = \chi_{KINETIC} + \chi_{DIRECT} + \chi_{EXCHANGE}$$

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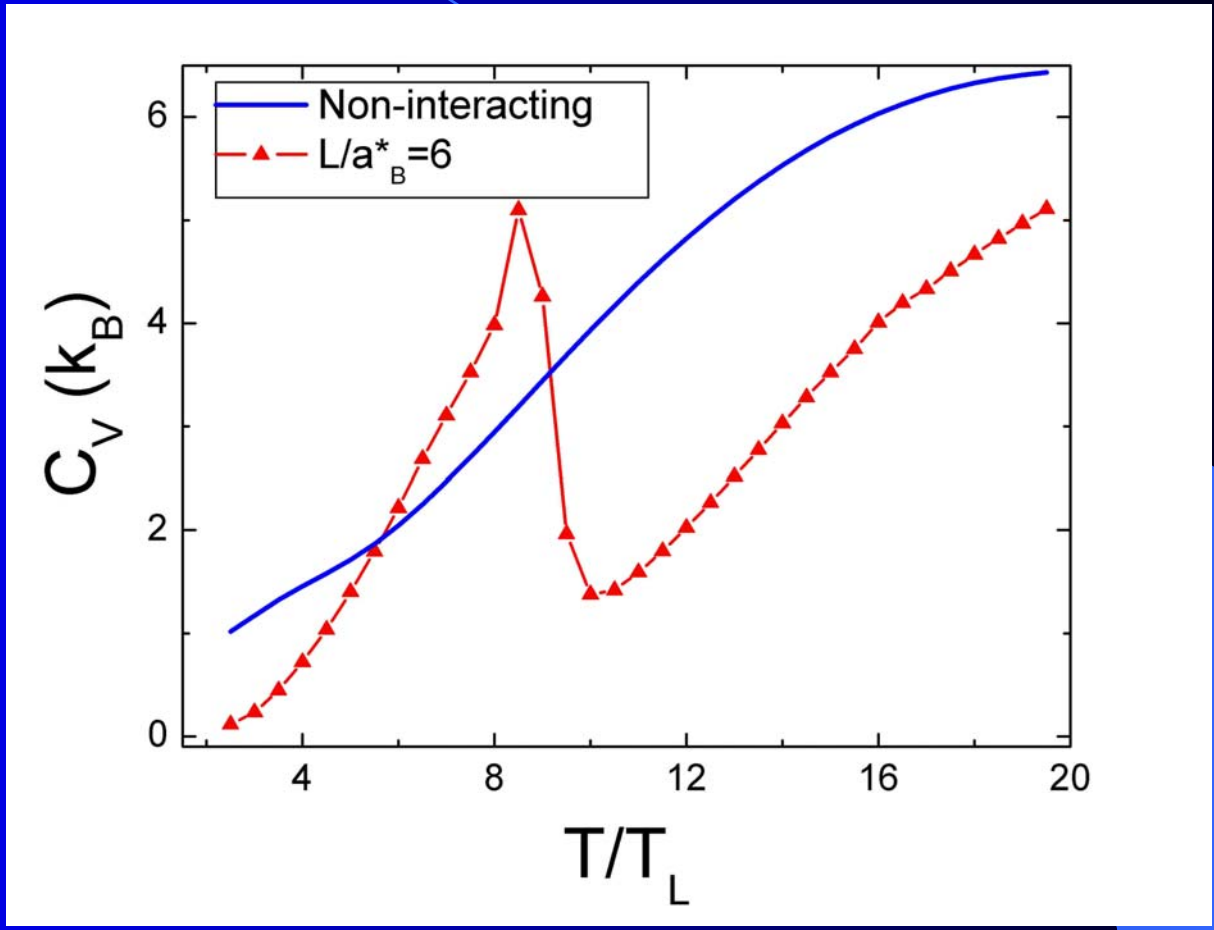
Specific Heat

$$C_v(T) = -\left(\frac{\partial U}{\partial T}\right)_V$$

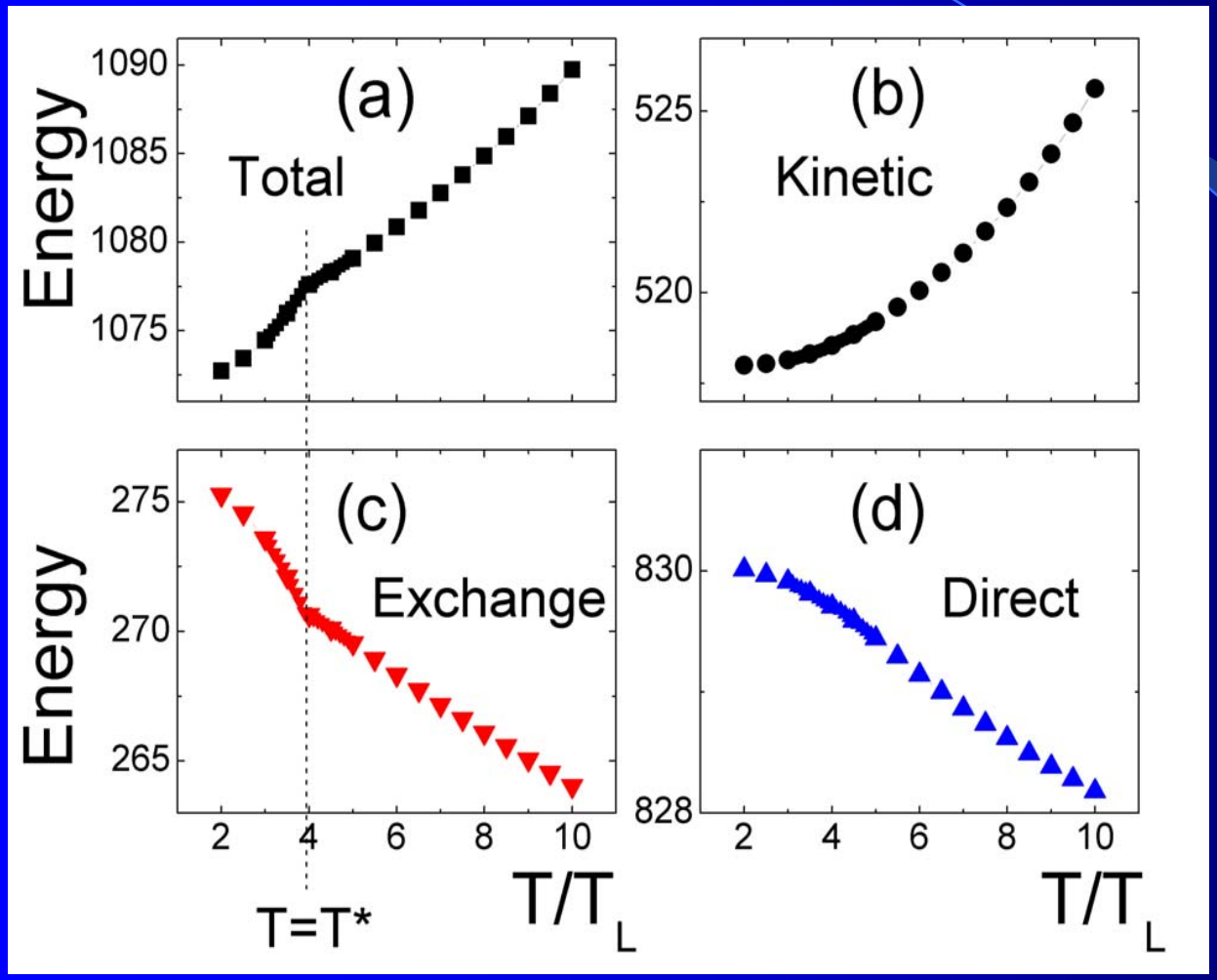
$$U \approx E_g^{HF}(T, N, r_s, B)$$

$$k_B T_L \equiv \hbar^2 / m^* L^2$$



Sharp drop in C_v : Phase transition ??

Transition is *Exchange*-induced



$$C_v(T) = -\left(\frac{\partial U}{\partial T}\right)_V$$

$$U \approx E_g^{HF}$$

$$E_g^{HF} = E_{kin} + E_D + E_X$$

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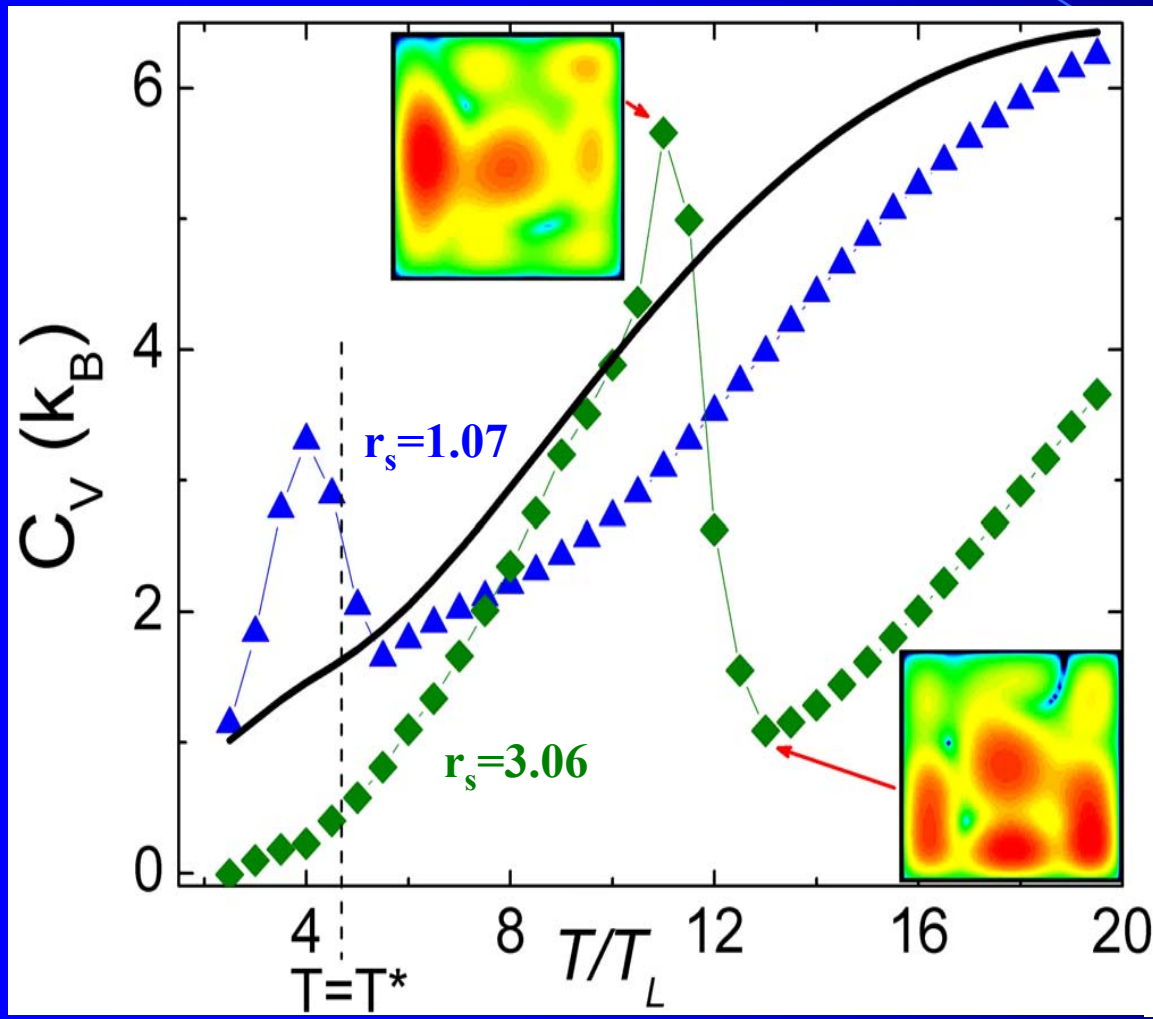
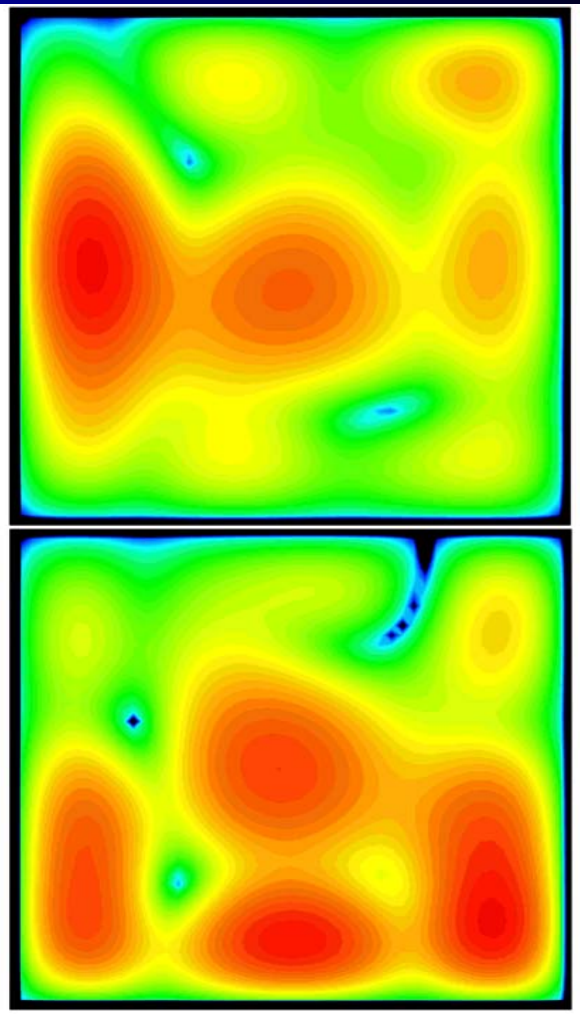
Exchange-induced phase transition





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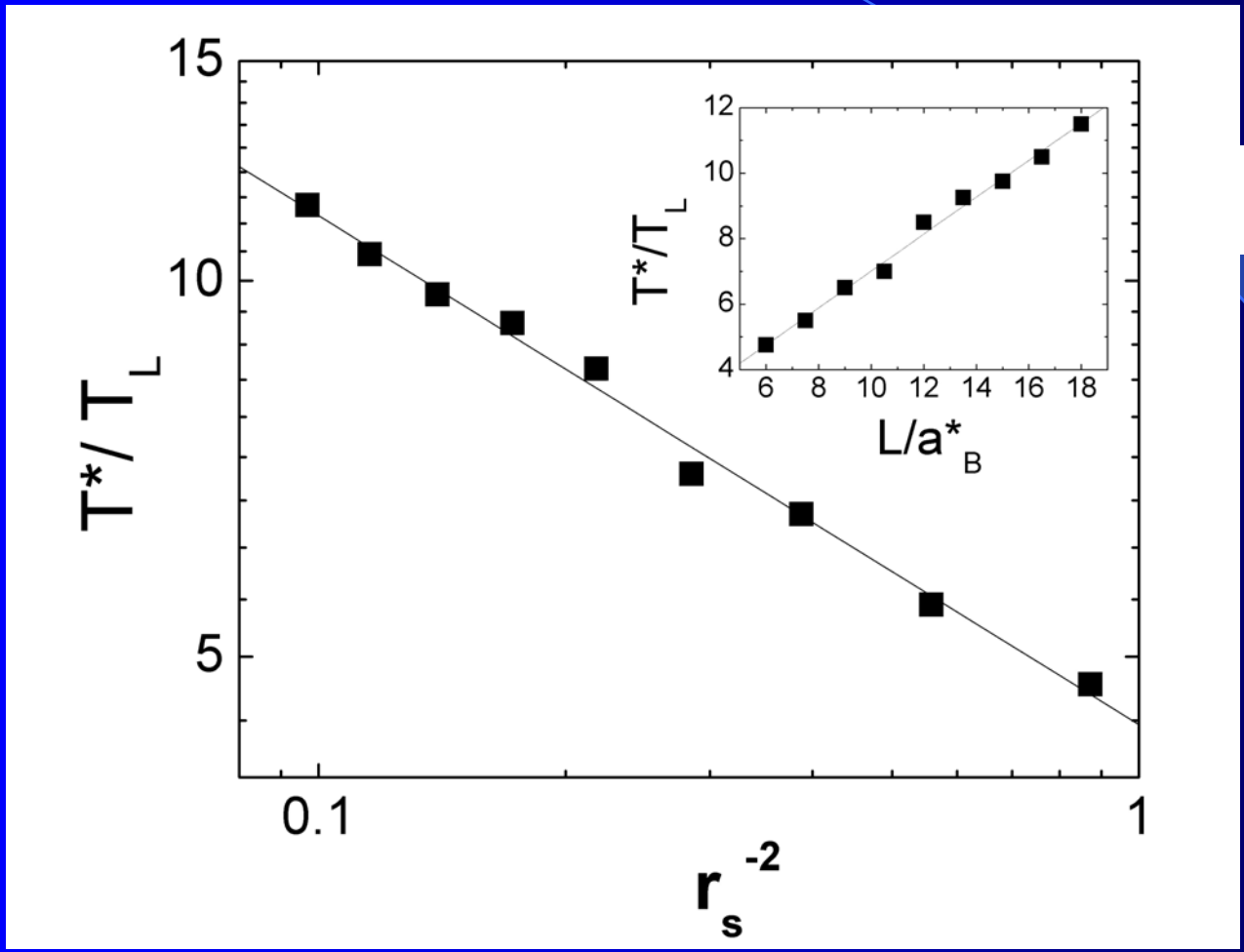
Transition temperature T^*

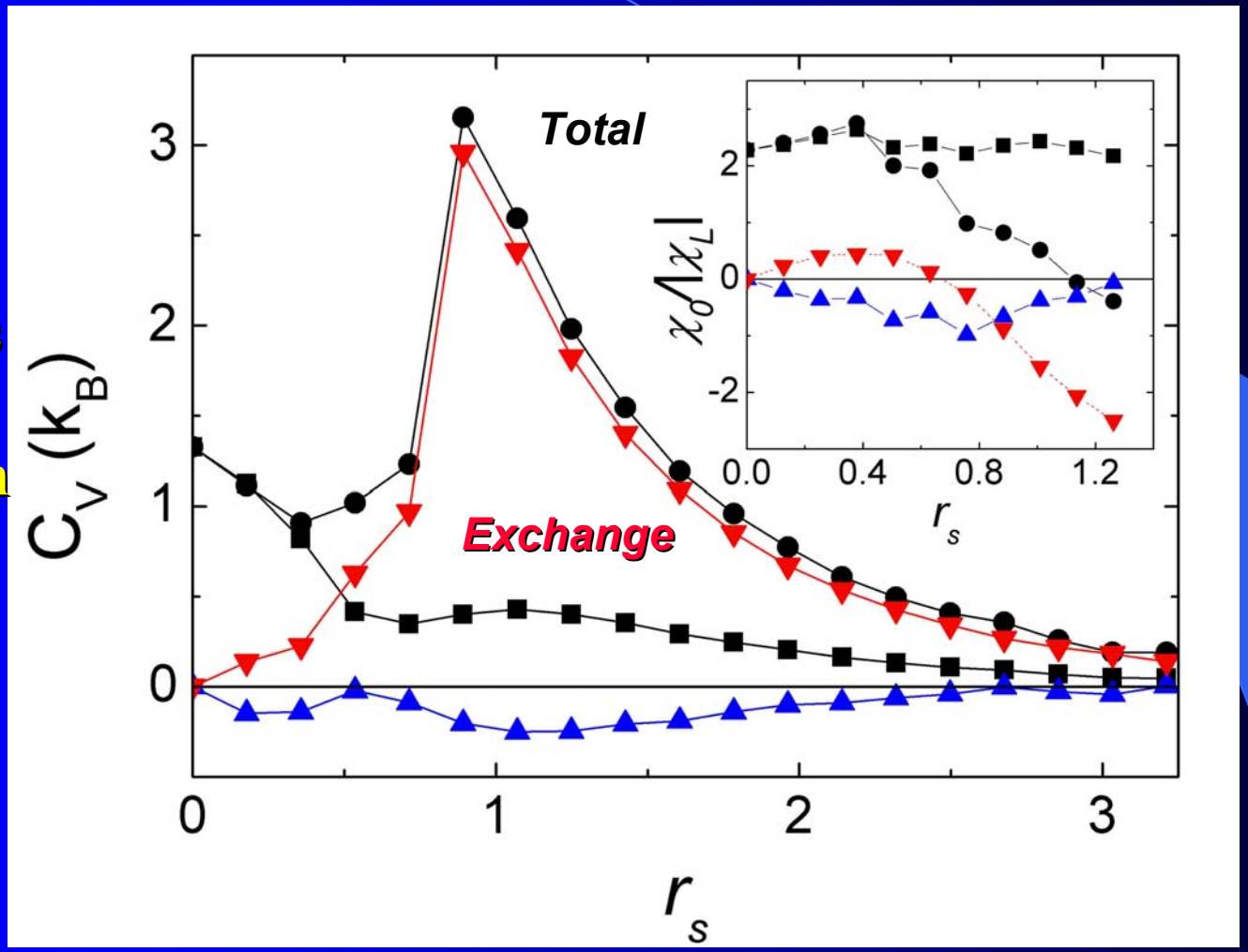


$$k_B T_L \equiv \hbar^2 / m^* L^2$$

GaAs QD w/ L=50 nm: T*~11 K (L=100 nm: T*~1 K)

Exchange term: leading contribution

Again: Exchange is the largest contribution for $r_s \sim 1$



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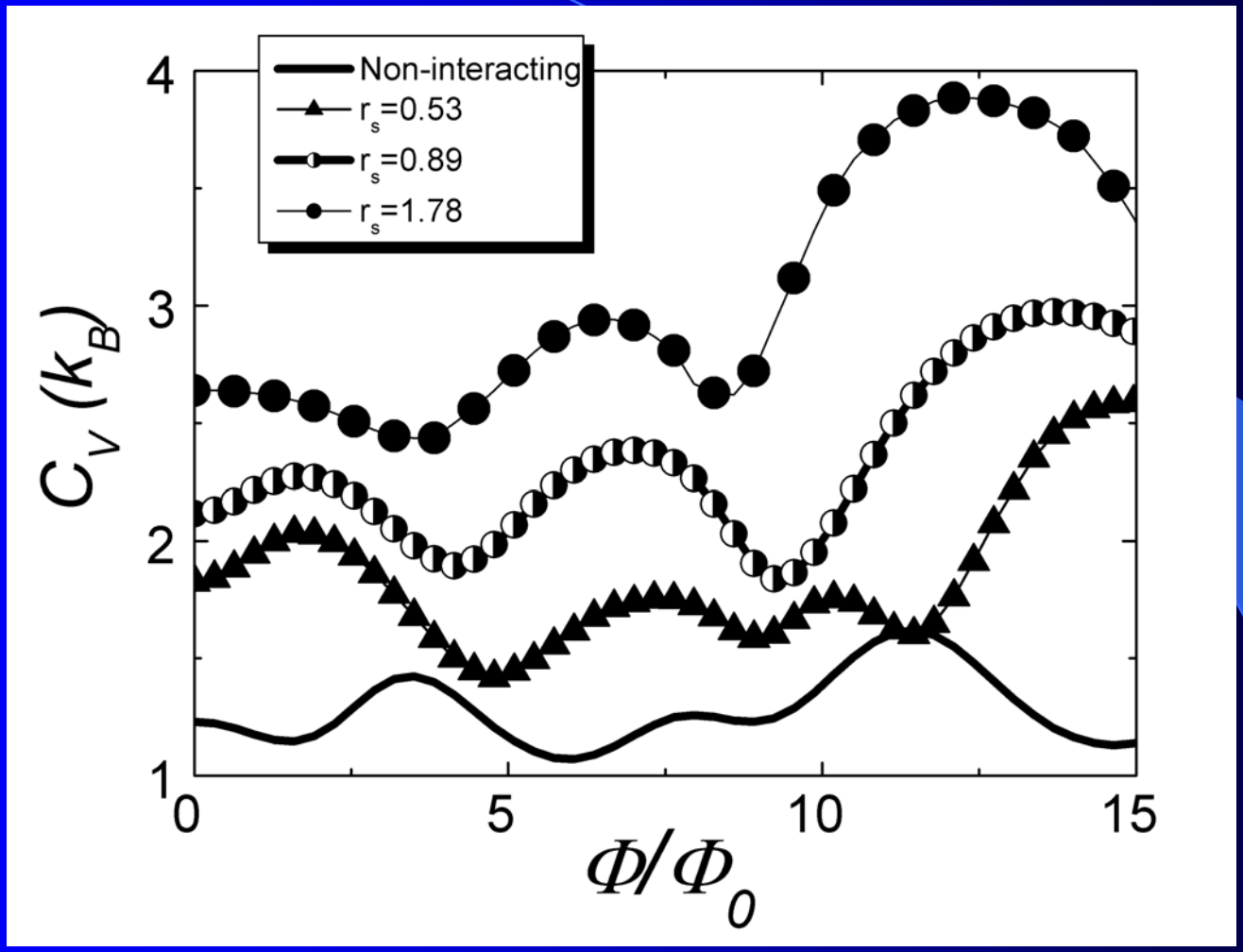
Oscillations with Magnetic Field



Interaction "removes Harmonics" from $C_v(B)$

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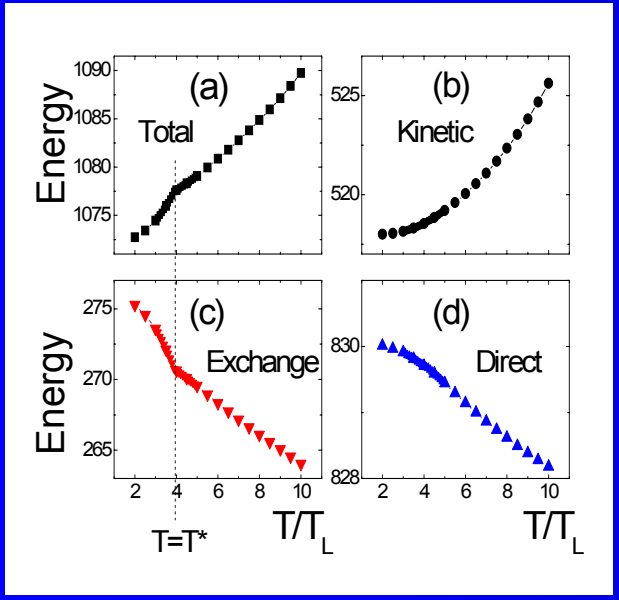
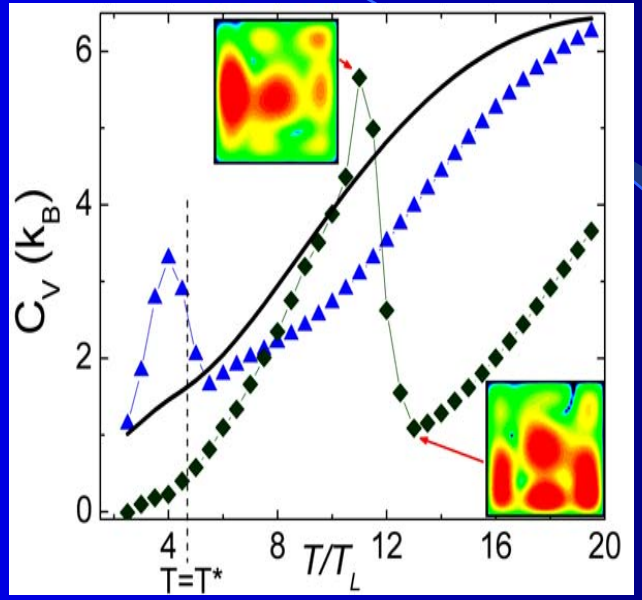
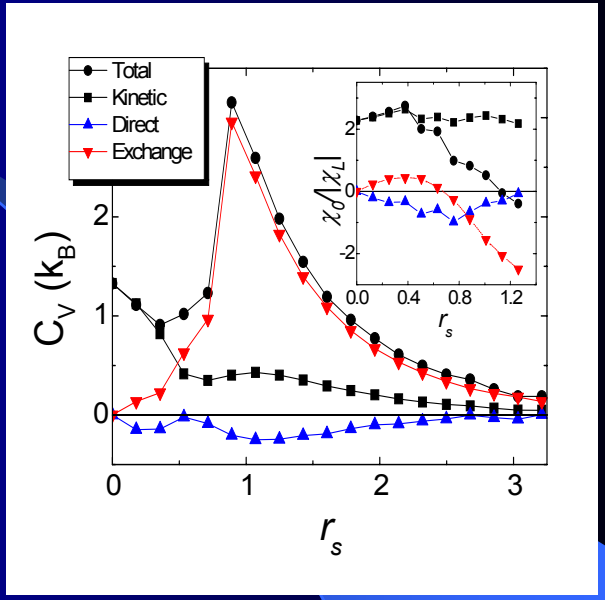
Conclusions: e-e interaction effects in the thermodynamics of QDs.







- Exchange (Fock) contribution to the many-body energy shows non-trivial temperature dependance.
- Exchange-induced discontinuities in $C_v(T=T^*)$: Charge phase transitions.
- $T^* \sim L^{-1}$
- Exchange dominates the thermodynamic properties in the r_s~1.5-2.0 range.

References: *PRB* **69** 075311 (2004); *PRB* **71** 113302 (2005).