Interaction Matrix Element Fluctuations

in Quantum Dots

Lev Kaplan

Tulane University

and

Yoram Alhassid

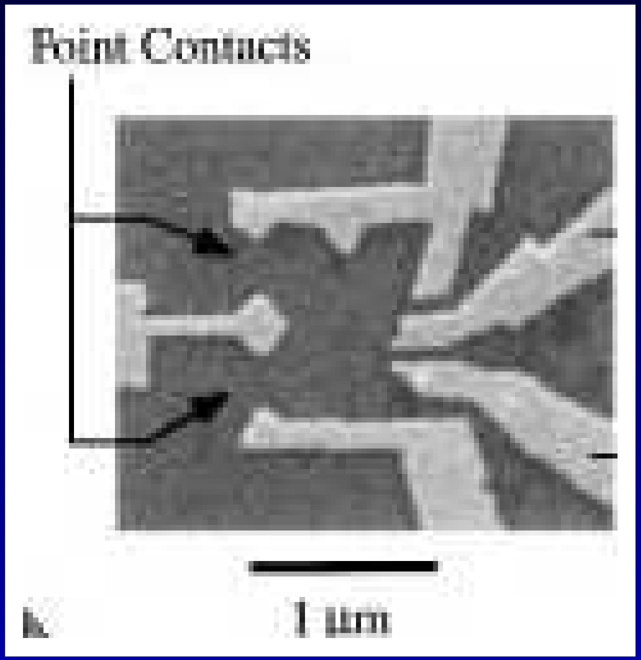
Yale University

Outline

- Ballistic dots in Coulomb blockade regime
  - Conductance peak spacings: need interactions
- Computing IMEs:
  - Relation to single-particle correlators
- Random wave model ($N \to \infty$)
- What happens in actual chaotic dots?
  - Failure of random wave model
  - Failure of leading-order semiclassical theory
  - Can we compute subleading terms in $1/N$?
  - Beyond chaos (time permitting)
- Summary

Coulomb Blockade Regime

- Dot weakly coupled to outside via two leads

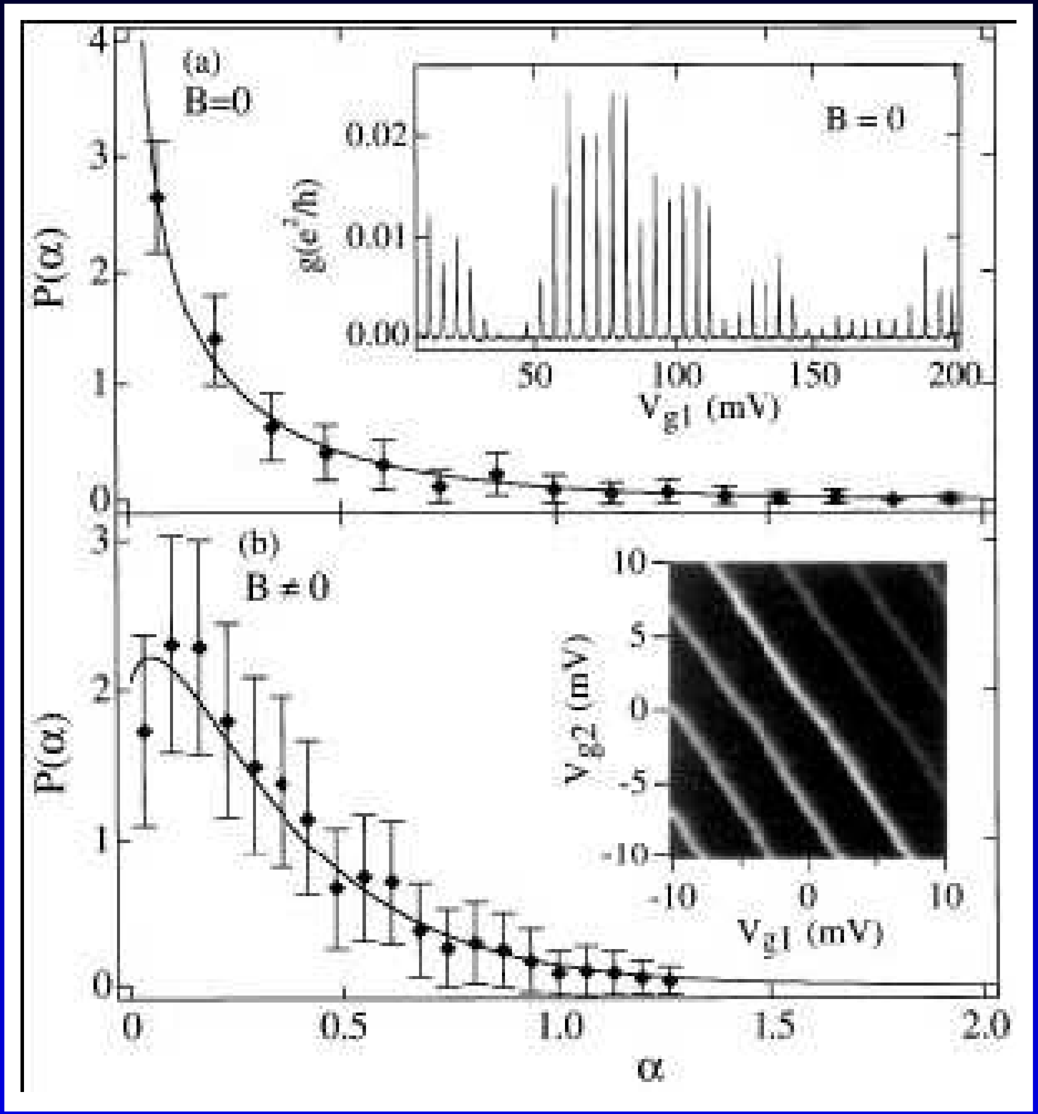


- Decay width $\ll$ Temperature $\ll$ Charging energy
- Sharp conductance peaks when Fermi energy in leads matches energy needed to move one new electron onto dot ($N \to N+1$)

Coulomb Blockade Regime

- Peaks depend on many-body energies E_N and associated wave functions
- E.g., peak spacings given by $E^{\text{gs}}_{N+1} - 2E^{\text{gs}}_N + E^{\text{gs}}_{N-1}$ for $T = 0$
- Statistical properties for $N \gg 1$?
- Hartree-Fock approach: E_N includes
  - Classical charging energy $N^2e^2/2C$
  - Constant exchange interaction
  - Mean-field single-electron potential (chaotic)
  - Residual two-electron interaction
  - Surface charge interaction

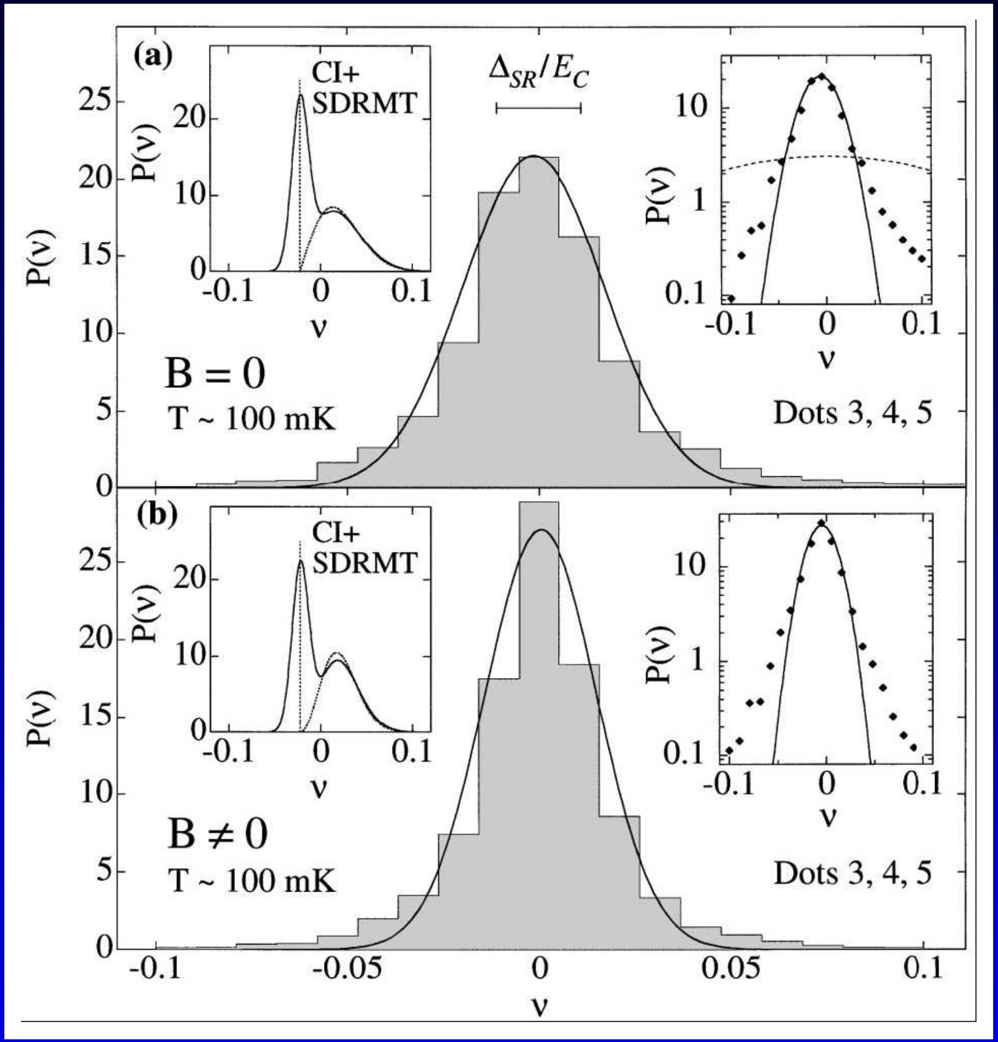
Peak Height Distribution



Folk et al, PRL (1996)

Peak height statistics well explained using constant interaction + chaotic mean field

Peak Spacing Distribution



Patel et al, PRL (1998)

Peak spacing distribution predicted to be bimodal ($e^2/C + \epsilon_{N+1} - \epsilon_N$ followed by e^2/C) in mean-field model (*not* observed)

Two-body interactions essential for understanding spacings

Interaction Matrix Elements

- Diagonal two-body IME $v_{\alpha\beta} \equiv v_{\alpha\beta;\alpha\beta}$
- Contact interaction model:

$$\boxed{v_{\alpha\beta} = V\Delta \int_V d\vec{r}\, |\psi_\alpha(\vec{r})|^2 \, |\psi_\beta(\vec{r})|^2}$$

- Interested in fluctuations $\overline{\delta v_{\alpha\beta}^2}$, etc.
- To leading order in $g_T \sim kL \sim \sqrt{N}$ $(L \equiv \sqrt{V})$,

$$\boxed{\overline{\delta v_{\alpha\beta}^2} = \Delta^2 V^2 \int_V \int_V d\vec{r}\, d\vec{r}'\, \tilde{C}^2(\vec{r}, \vec{r}') + \cdots}$$ where

$$\tilde{C}(\vec{r}, \vec{r}') = \overline{|\psi(\vec{r})|^2 |\psi(\vec{r}')|^2} - \overline{|\psi(\vec{r})|^2}\ \overline{|\psi(\vec{r}')|^2}$$

Interaction Matrix Elements

- Similar expressions for
  - variances $\overline{\delta v_{\alpha\alpha}^2}$, $\overline{\delta v_{\alpha\beta\gamma\delta}^2}$
  - covariance $\overline{\delta v_{\alpha\beta}\,\delta v_{\alpha\gamma}}$ (relevant for spectral scrambling)
  - surface charge IME fluctuation $\overline{\delta v_{\alpha}^2}$
- Higher moments $\overline{\delta v^n}$ for $n \geq 3$ require $\tilde{C}(\vec{r}, \vec{r}', \vec{r}'')$ etc.
- Aside: IME distributions essential in diverse physical contexts, e.g., mode competition in micron- sized asymmetric dielectric laser resonators (Tureci & Stone)

Random wave model (Berry)

- Typical trajectory in classically ergodic system uniformly explores energy hypersurface
- Typical single-electron wave function should be composed of random superposition of basis states at fixed energy (e.g., plane waves in hard-wall billiard)
  - Gaussian-distributed $\psi(\vec{r})$
  - Free-space intensity correlation

$$C(\vec{r},\vec{r}') = \frac{2}{\beta}\frac{1}{V^2}J_0^2(k|\vec{r}-\vec{r}'|)$$

Random wave model: normalize

- Normalization in finite volume:

$$\begin{aligned}\tilde{C}(\vec{r},\vec{r}') &= C(\vec{r},\vec{r}') - \frac{1}{V}\int_V d\vec{r}_a\, C(\vec{r},\vec{r}_a)\\ &- \frac{1}{V}\int_V d\vec{r}_a\, C(\vec{r}_a,\vec{r}')\\ &+ \frac{1}{V^2}\int_V\int_V d\vec{r}_a\, d\vec{r}_b\, C(\vec{r}_a,\vec{r}_b) + \cdots\end{aligned}$$

- Satisfies $\int_V d\vec{r}'\, \tilde{C}(\vec{r},\vec{r}') = 0$ (Mirlin)

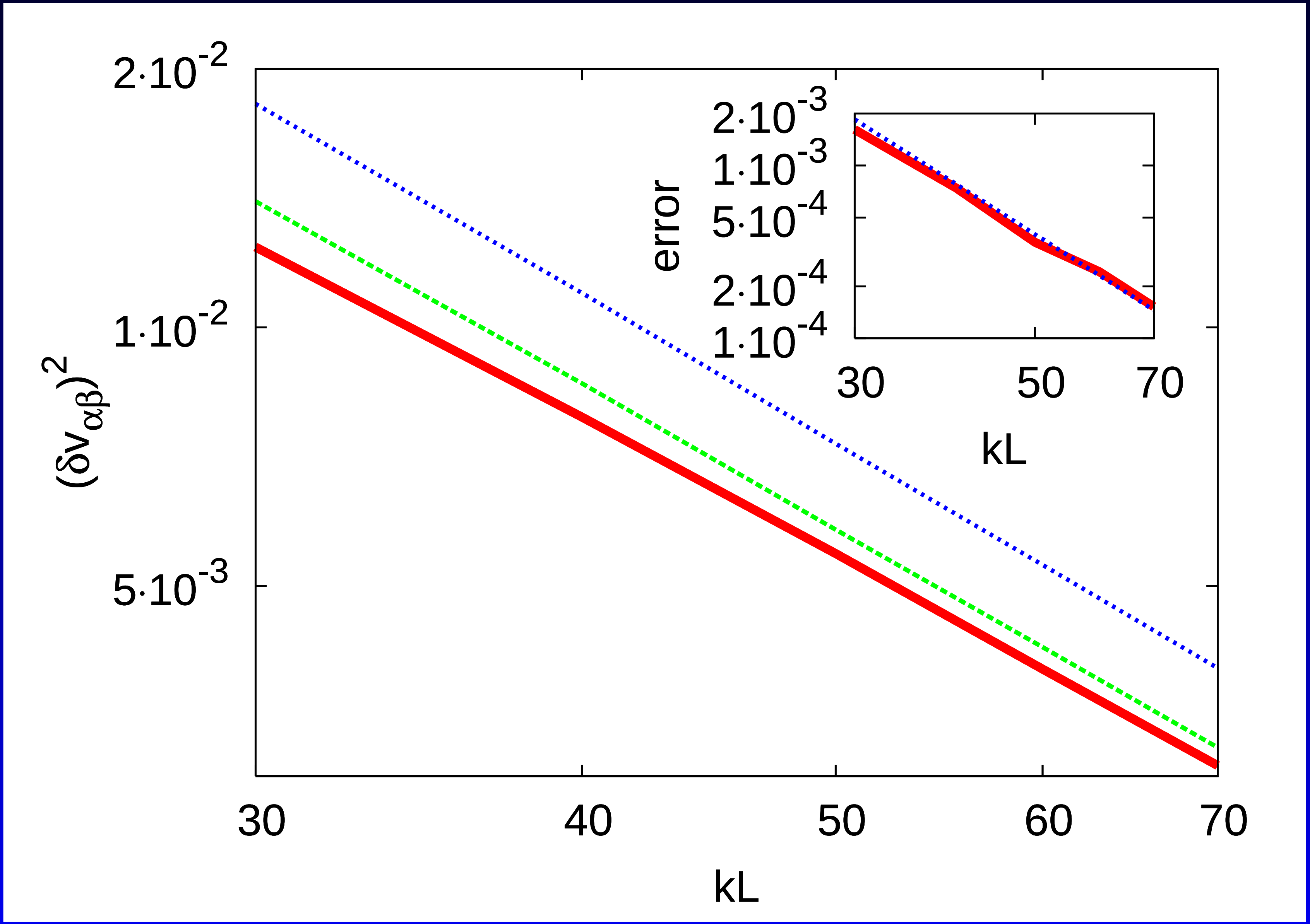
$$\Rightarrow \overline{\delta v_{\alpha\beta}^2} = \Delta^2 \frac{3}{\pi}\left(\frac{2}{\beta}\right)^2 \left[\frac{\ln kL + b_g}{(kL)^2} + O\left(\frac{1}{(kL)^3}\right)\right]$$

Random wave model: variance

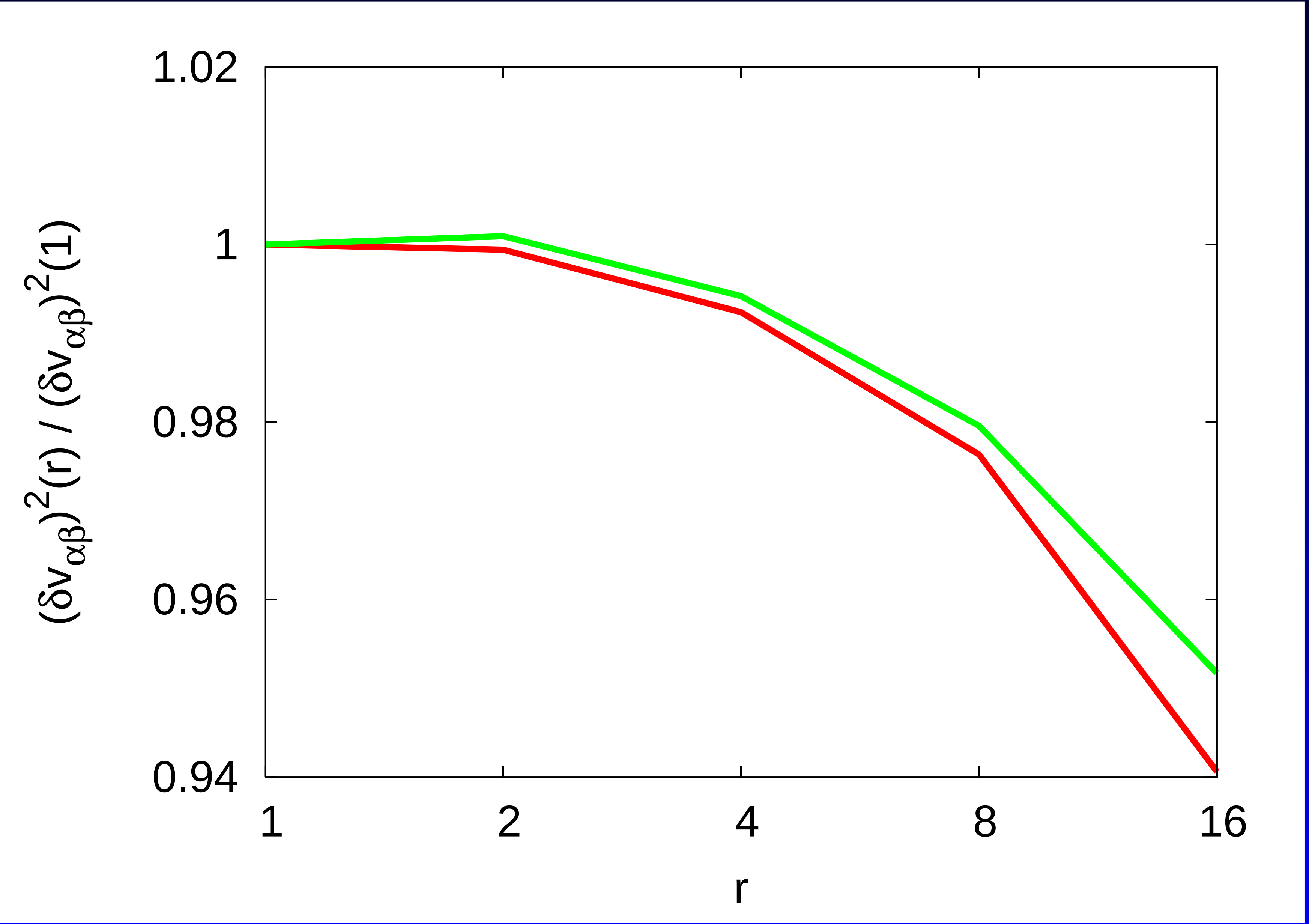
$$\overline{\delta v_{\alpha\beta}^2} = \Delta^2 \frac{3}{\pi} \left(\frac{2}{\beta}\right)^2 \left[\frac{\ln kL + b_g}{(kL)^2} + O\left(\frac{1}{(kL)^3}\right)\right]$$

- Leading $\ln kL/(kL)^2$ term depends only on symmetry class, normalization unnecessary
- b_g requires *normalized* correlator $\tilde{C}(\vec{r}, \vec{r}')$
- Shape dependence of b_g is weak ($< 5\%$)
- Subleading $O(1/(kL)^3)$ corrections are $< 10\%$ for systems of experimental interest

Subleading effects are small



Weak shape dependence of $\overline{\delta v^2_{\alpha\beta}}$



Random wave model

- Within random wave model, other matrix elements differ only by combinatoric factors *at leading order*

$$\overline{\delta v^2_{\alpha\beta}} = \Delta^2 \frac{3}{\pi} \left(\frac{2}{\beta}\right)^2 \left[\frac{\ln kL + b_g}{(kL)^2} + O\left(\frac{1}{(kL)^3}\right)\right]$$

$$\overline{\delta v^2_{\alpha\alpha}} = \Delta^2 \frac{3}{\pi} c_\beta \left[\frac{\ln kL + b'_g}{(kL)^2} + O\left(\frac{1}{(kL)^3}\right)\right]$$

$$\overline{\delta v^2_{\alpha\beta\gamma\delta}} = \Delta^2 \frac{3}{\pi} \left[\frac{\ln kL + b''_g}{(kL)^2} + O\left(\frac{1}{(kL)^3}\right)\right]$$

Matrix element distributions

- Naively, should be Gaussian (central limit theorem)
- Recall $\overline{\delta v_{\alpha\beta}^2} \sim \int_V \int_V d\vec{r}\, d\vec{r}'\, \tilde{C}^2(\vec{r}, \vec{r}') \sim \frac{\Delta^2 \ln kL}{(kL)^2}$
- Similarly $\overline{\delta v_{\alpha\beta}^3} \sim \int_V \int_V \int_V d\vec{r}\, d\vec{r}'\, d\vec{r}''\, C^2(\vec{r}, \vec{r}', \vec{r}'')$

  where $C(\vec{r}, \vec{r}', \vec{r}'') \sim c_{3\beta}\, J_0(k|\vec{r} - \vec{r}'|)$

  $$\times J_0(k|\vec{r}' - \vec{r}''|) J_0(k|\vec{r}'' - \vec{r}|) + \cdots$$
- Thus $\overline{\delta v_{\alpha\beta}^3} = b_{3g}\, c_{3\beta}^2\, \frac{\Delta^3}{(kL)^3}$
  - b_{3g} is geometry-dependent constant
  - $c_{3\beta}$ is combinatoric factor
  - Note: no logarithmic divergences

Matrix element distributions

- Skewness $\gamma_1 = \overline{\delta v^3_{\alpha\beta}} \;/\; \left[\, \overline{\delta v^2_{\alpha\beta}} \,\right]^{3/2}$

$$\boxed{\gamma_1 = b_{3g}\; c^2_{3\beta} \left(\frac{\beta}{2}\right)^3 \left(\frac{\pi}{3}\right)^{3/2} (\ln kL)^{-3/2} + \cdots}$$

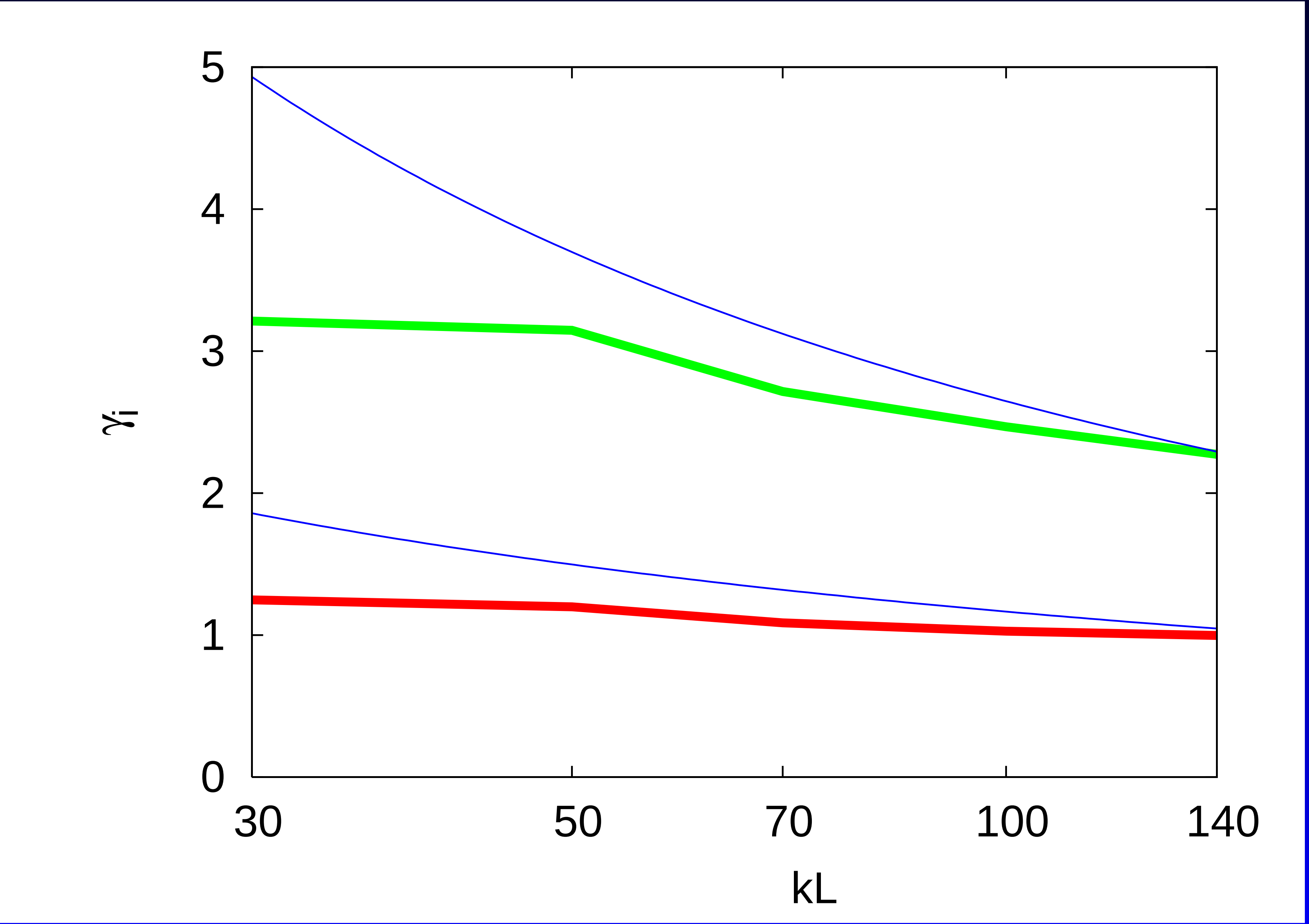
- Excess kurtosis

$$\gamma_2 = \left(\overline{\delta v^4_{\alpha\beta}} - 3 \left[\, \overline{\delta v^2_{\alpha\beta}} \,\right]^2 \right) \;/\; \left[\overline{\delta v^2_{\alpha\beta}} \,\right]^2$$

$$\boxed{\gamma_2 = b_{4g} \left(c^2_{4\beta} + \left(\frac{2}{\beta}\right)^4 \right) \left(\frac{\pi^2}{3}\right) (\ln kL)^{-2} + \cdots}$$

- Very slow convergence of interaction matrix elements to Gaussian statistics even for Gaussian random single-electron wave functions

Skewness and excess kurtosis

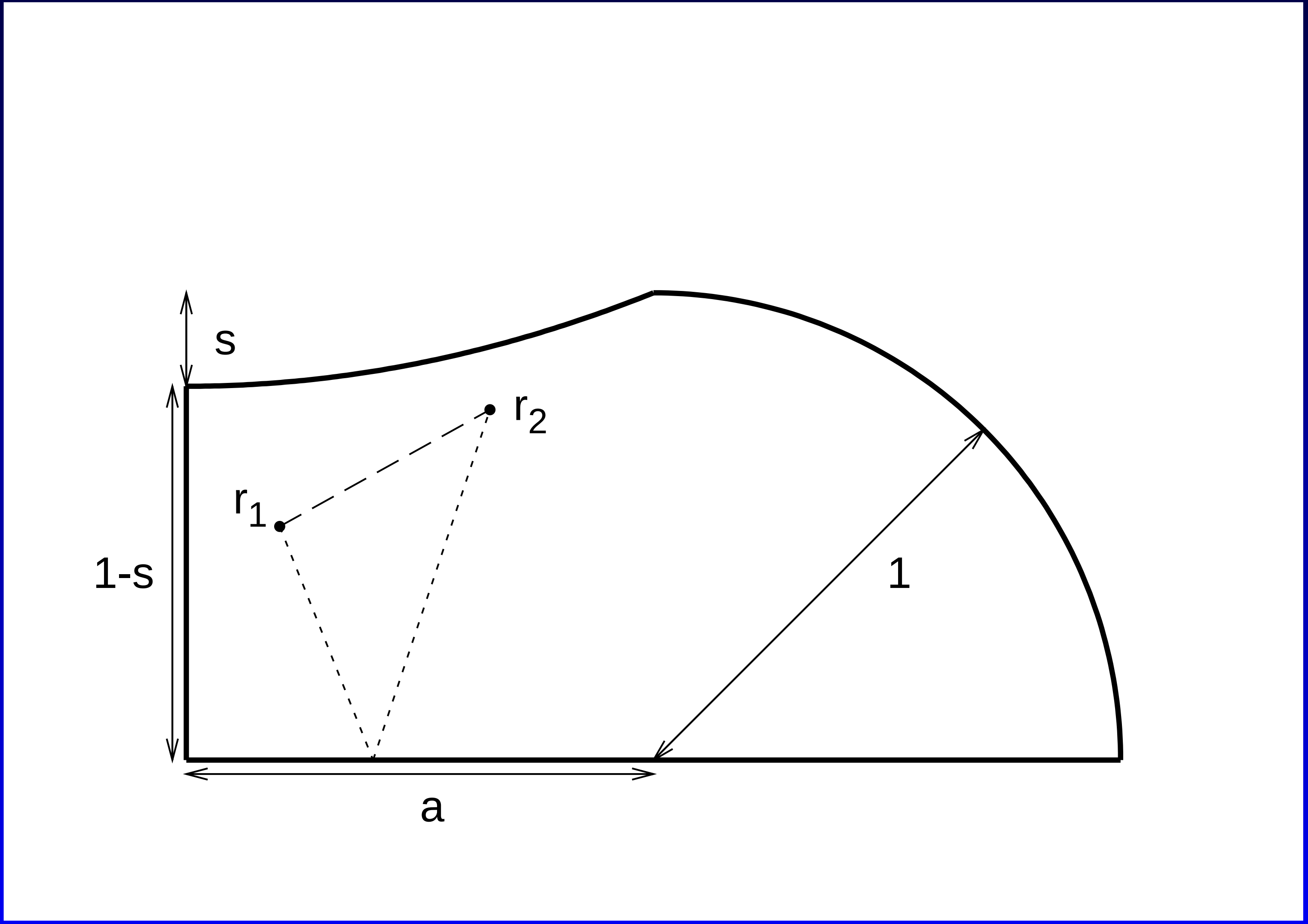


What do we have so far?

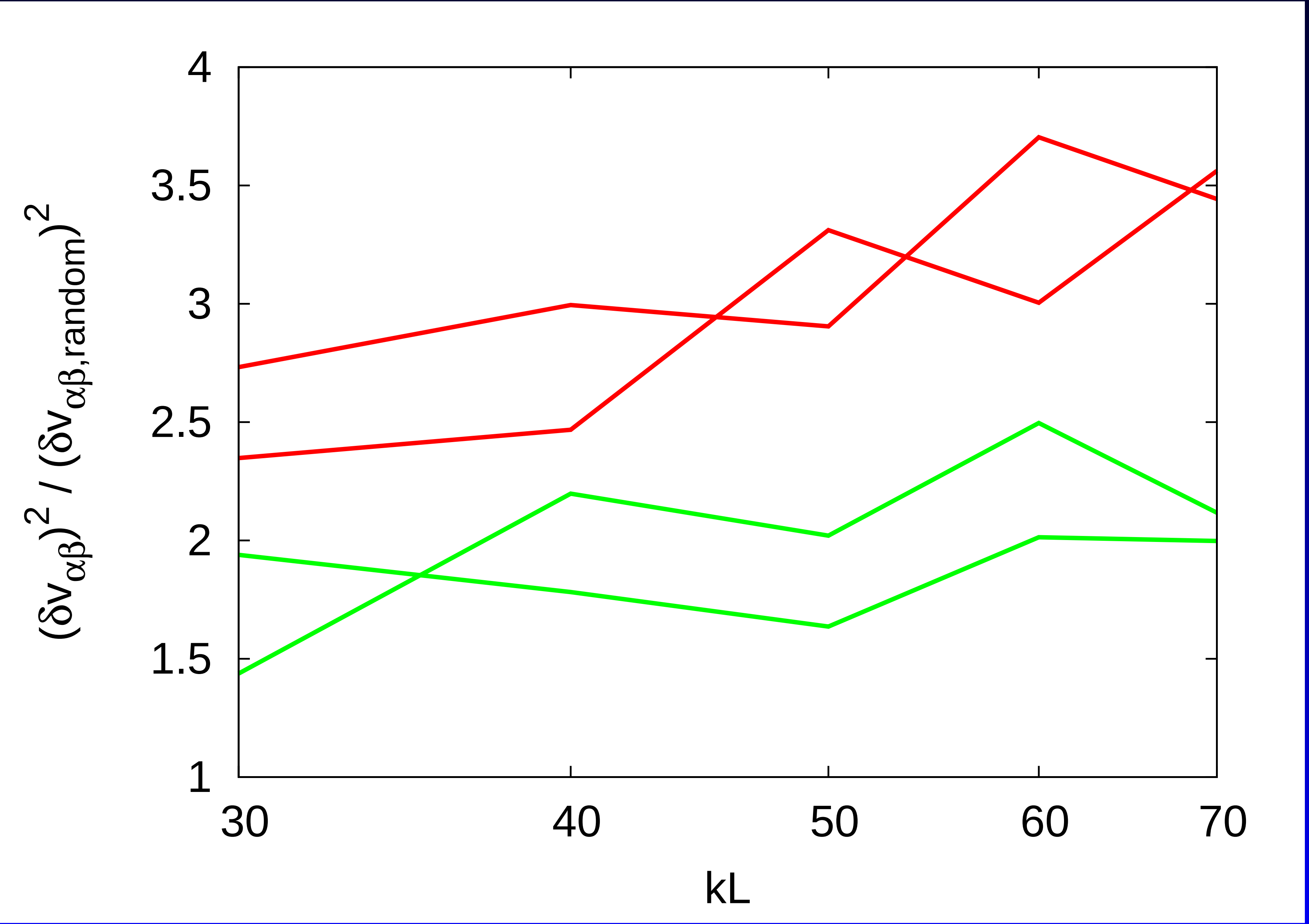
- Can use quantum chaos methods to compute universal IME distribution as function of single semiclassical parameter kL
- Unfortunately, distribution is too narrow to be consistent with low-temperature experimental data on peak spacings
- Brings into question validity of Hartree-Fock?

Actual chaotic systems

Example: modified quarter-stadium billiard



Variance enhancement over RW



Actual chaotic systems: results

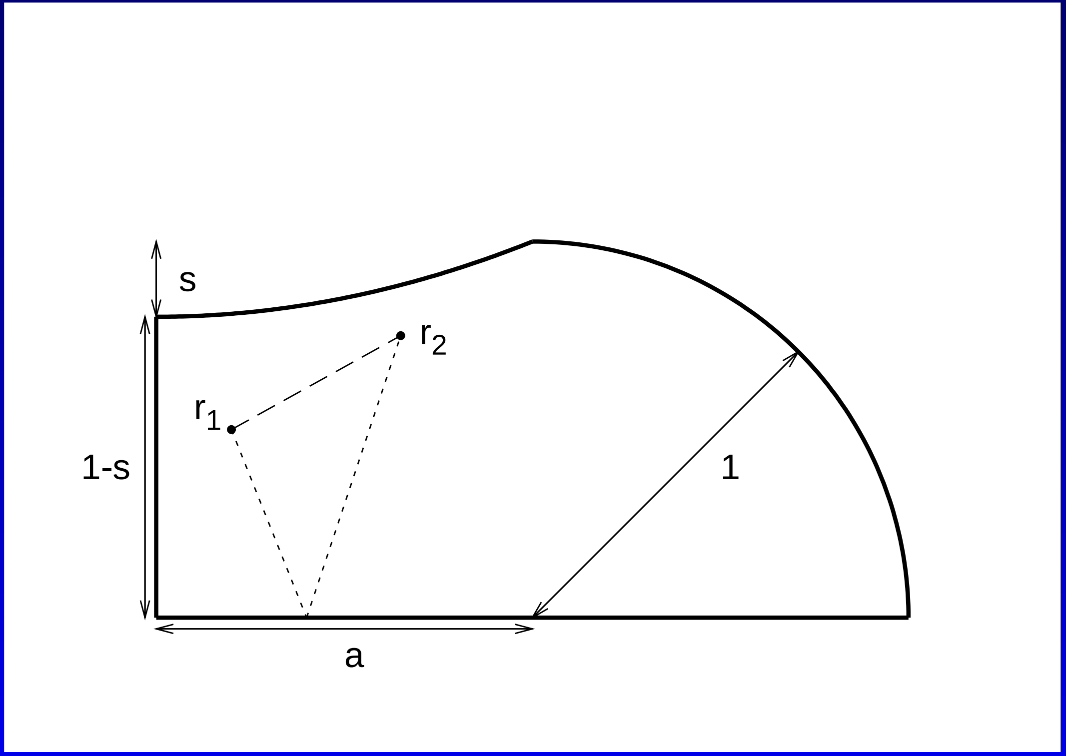
- $v_{\alpha\beta}$ variance enhanced by 2 – 4 over random wave predictions for $kL \sim 50$ to 70
- Robust to moderate shape changes
- No apparent convergence with increasing kL (!)
- Good: Increased fluctuations consistent with experimental data at low temperatures
- Good: Support for validity of Hartree–Fock
- Bad: Discrepancy with well-established random wave model
- $\Rightarrow$ Better understanding needed of actual chaotic billiards

Actual chaotic systems: results

- Relation $\boxed{\overline{\delta v^2_{\alpha\beta}} = \Delta^2 V^2 \int_V \int_V d\vec{r}\, d\vec{r}'\, \tilde{C}^2_{\rm bill}(\vec{r},\vec{r}')}$ still holds
  - $\tilde{C}^2_{\rm bill}(\vec{r},\vec{r}')$ = intensity correlator for actual billiard (not random waves)
- Large observable effects on behavior associated with interactions come from subtle correlations within single-particle states
  - How to calculate these correlations?
  - Try semiclassical approach ...

Semiclassical calculations

- Correlation $C(\vec{r}, \vec{r}')$ in RW model arises from straight-line path connecting $\vec{r}$ and $\vec{r}'$
- Additional correlation terms from bouncing paths (Hortikar & Srednicki, Urbina & Richter)



Semiclassical calculations

- Intensity correlator:

$$C_{\rm sc}(\vec{r},\vec{r}') = \frac{1}{V^2}\frac{2}{\beta}\left[J_0^2(k|\vec{r}-\vec{r}'|) + O\left(\frac{T_{\rm clas}}{T_B}\frac{1}{kL}\right)\right]$$

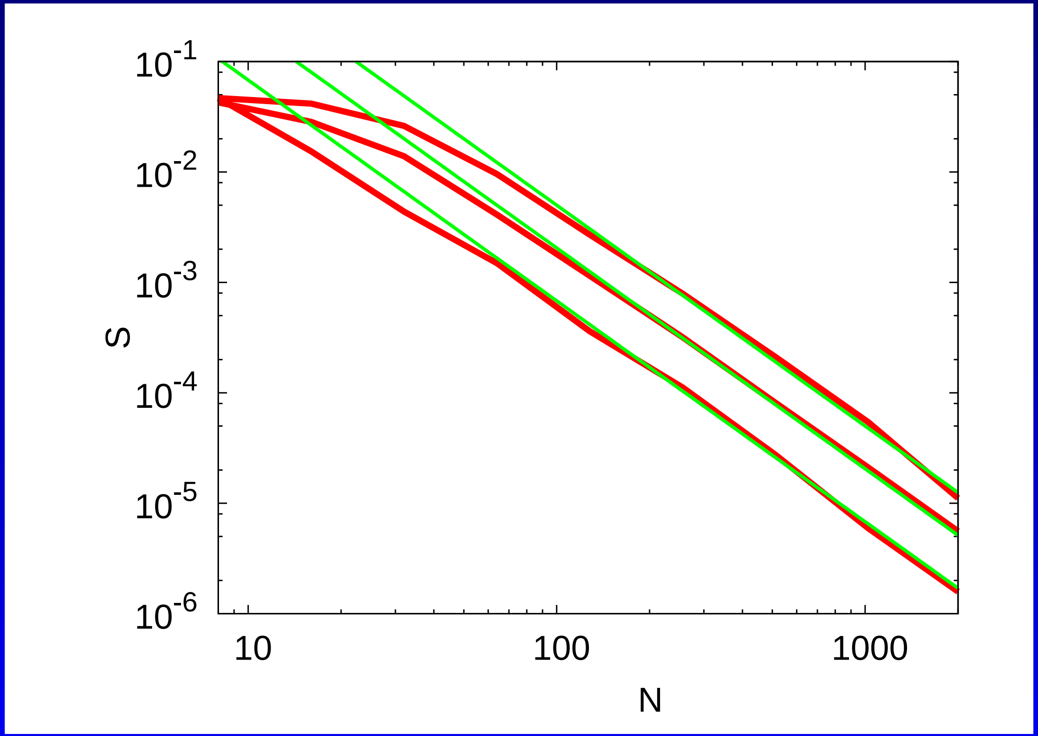
- $T_{\rm clas}/T_B =$ correlation time / bounce time

$$\boxed{\overline{\delta v_{\alpha\beta}^2} = \Delta^2 \frac{3}{\pi}\left(\frac{2}{\beta}\right)^2 \left[\frac{\ln kL + b_g + b_{\rm sc}}{(kL)^2} + O\left(\frac{1}{(kL)^3}\right)\right]}$$

- $b_{\rm sc}$: formally $\sim T_{\rm clas}^2/T_B^2$; in practice, typically large and overwhelms universal $\ln kL$

Semiclassical calculations

- Semiclassically predicted scaling not observed at all for $kL \leq 100$
  - Reason: Formally subleading $O(1/(kL)^3$ and higher-order terms comparable to leading one
  - Numerical confirmation: quantum maps

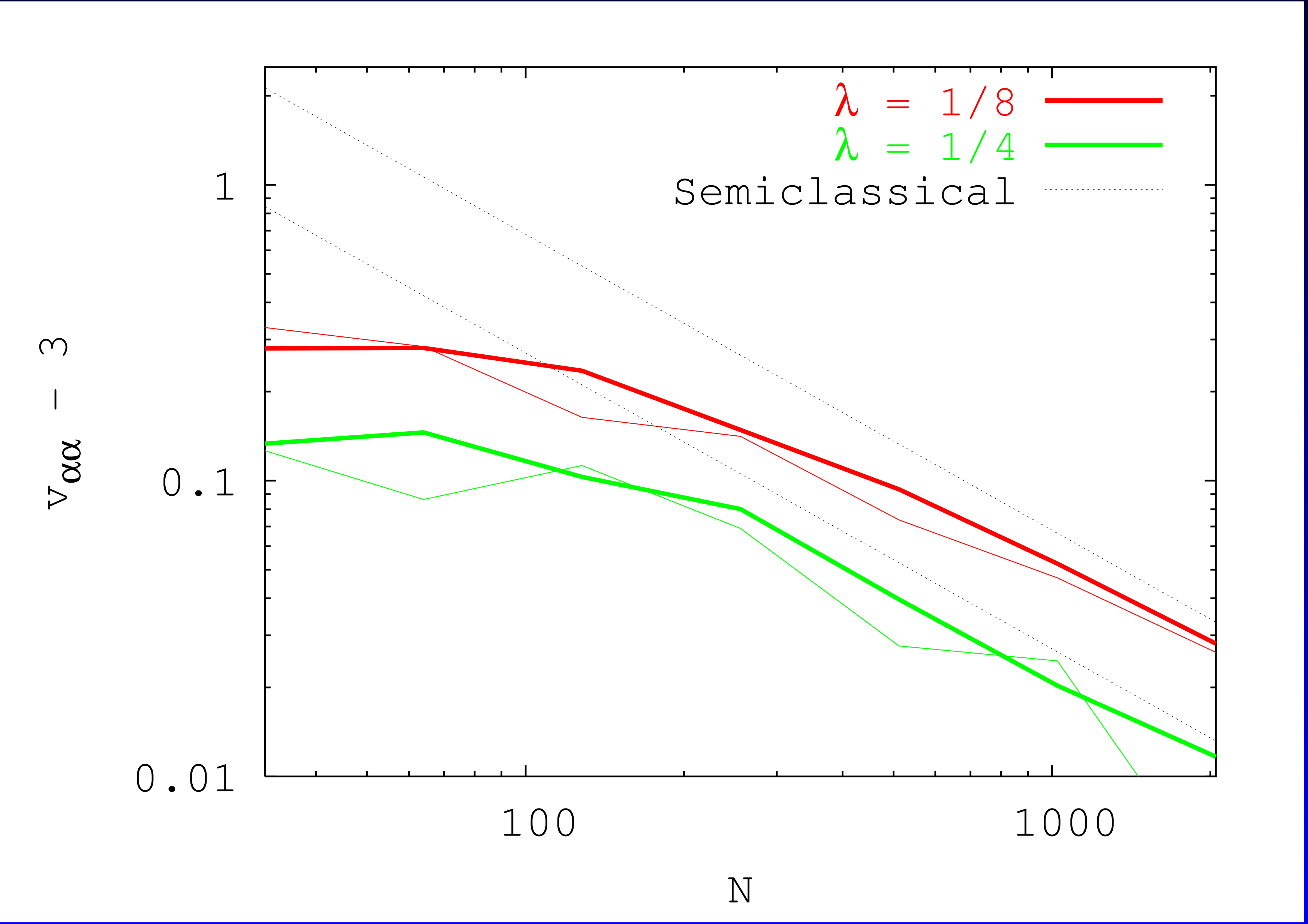


Short-time calculations (with Matthew Smith)

- Naive semiclassical expressions do not work
- Nevertheless, we expect (or hope) that IME statistics can be reliably computed using short-time information (few bounces)
  - To have predictive power, statistics must depend only on coarse-scale geometry
  - Confirmed by robustness of results for perturbed modified stadium billiards
- In maps, $\overline{v_{\alpha\alpha}}$ (=IPR) may be reliably computed using

$$\overline{v_{\alpha\alpha}} = v_{\alpha\alpha,\,\mathrm{RMT}} \frac{\sum_{t=-T}^{T} |\langle\alpha|\alpha(t)\rangle|^2}{\sum_{t=-T}^{T} |\langle\alpha|\alpha(t)\rangle|^2_{\mathrm{RMT}}}$$

Short-time calculations of $\overline{v_{\alpha\alpha}}$



Summary

- Observable properties of interacting system computable in terms of single-electron wave function correlations
- Simple expressions for IME fluctuations in random wave limit
- Non-Gaussian distribution of IMEs
- Failure of random wave picture for experimentally relevant system sizes
  - Underestimates $v_{\alpha\beta}$ variance by factor of $3 – 4$
  - Discrepancy even greater for $B \neq 0$
  - Predicts wrong sign for covariance, $v_{\alpha\alpha} - 3$

Summary

- Dynamical effects essential to obtain agreement with experiment
  - Inadequacy of leading-order semiclassics for computing these effects
  - Hope for robust predictions using short-time dynamics combined with long time RMT