Semiclassical theory of non-local statistical measures: residual Coulomb interactions

Steve Tomsovic\textsuperscript{1}, Denis Ullmo\textsuperscript{2}, and Arnd Bäcker\textsuperscript{3}

\textsuperscript{1}Washington State University, Pullman
\textsuperscript{2} Laboratoire de Physique Théorique et Modèles Statistiques, Orsay
\textsuperscript{3} Technische Universität Dresden

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Today’s thread of logic

- Motivating non-local statistical measures
  - Quantum dots
  - Ground state energy shifts from residual interactions
- Random plane wave modeling
  - Normalization
  - Averages
  - Fluctuations
- Semiclassical theory
  - Bogomolny revisited
  - Chaotic quantum billiards
  - Periodic orbit spectrum
  - Deficiencies of random plane waves
  - Non-chaotic systems
- Outlook
Quantum dot illustration

Christian Schönenberger, University of Basel

http://pages.unibas.ch/phys-meso/Pictures/pictures.html

- Interested in a quantum dot holding on the scale of a hundred to a few hundreds of electrons
- Also interested in the entrance and exit leads being so narrow as to require tunneling on and off, i.e. a nearly isolated dot
- Can speak of the many-body energy levels, ground state, etc...

\[
E_{gr}[N] = \frac{e^2 N^2}{2C} + \sum_{i,\sigma} f_i^\sigma \epsilon_i + E_{ri}
\]
An aside

- Peak heights are correlated!
- Narimanov et al, PRL 1999 & PRB 2001 - periodic orbits induce correlations

Folk et al., PRL 1996
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Quantum dots
Residual interaction energy shifts

A comment

Ullmo et al., PRL 2003
Chaotic billiard models

cardioid billiard
purely chaotic
Dirichlet boundary conditions, entire boundary

stadium billiard
purely chaotic, but has bouncing ball modes
partial Dirichlet and Neumann boundary conditions
Consider the short-range screened Coulomb interaction:

\[ V_{sc}(\mathbf{r} - \mathbf{r}') = \frac{F_0}{\nu} \delta(\mathbf{r} - \mathbf{r}') \]

First order perturbation theory corrects the ground state energy by an amount:

\[ E^{RI} = \frac{F_0^a}{\nu} \int d\mathbf{r} n_{\uparrow}(\mathbf{r}) n_{\downarrow}(\mathbf{r}) = \frac{F_0^a A \Delta}{2} \sum_{i,j} f_i,(+) f_j,(-) \int d\mathbf{r} |\psi_i(\mathbf{r})|^2 |\psi_j(\mathbf{r})|^2 \]

But, the ground state is the minimum of the various configurations of occupied levels and the quantity

\[ S_i = A \sum_{j=1}^{i} \int d\mathbf{r} |\psi_i(\mathbf{r})|^2 |\psi_j(\mathbf{r})|^2 \]

determines roughly whether one configuration or another with one particle displaced has the lower energy.
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\( S_i \) component parts

- \( S_i \) – think of as being comprised of two component parts

\[
S_i = \mathcal{A} \int \mathrm{d}r \ |\Psi_i(r)|^2 \sum_{j \leq i} |\Psi_j(r)|^2 = \mathcal{A} \int \mathrm{d}r \ |\Psi_i(r)|^2 N(r; E_i^+) \\
N(r, E_i^+) = (\text{Friedel-like osc.}) + \text{tiny fluctuations}
\]

- The other component, \( |\Psi_i(r)|^2 \), is often taken statistically to be a random wave field
Random plane waves in the neighborhood of the boundary (using locally defined coordinates):

$$\psi_i(r) = \frac{1}{N_{\text{eff}}} \sum_{l=1}^{N_{\text{eff}}} a_l \text{cs} (k_l \cdot \hat{x}) \cos (k_l \cdot \hat{y} + \varphi_l)$$

$$1 = \int \text{d}r \left\langle |\psi_i(r)|^2 \right\rangle = \frac{\sigma^2}{4N_{\text{eff}}} \int \text{d}r \left[ 1 \pm J_0(2k_F x) \right] = \frac{A\sigma^2}{4N_{\text{eff}}} \left( 1 \pm \frac{L}{2k_F A} \right)$$

Approximation for the Friedel-like oscillations

$$N(r; E_i^+) = \frac{i}{\mathcal{A}} \left[ 1 \pm \frac{J_1(2k_ir)}{k_ir} \right] + \delta N(r; E_i^+)$$
It is advantageous to split the eigenfunction into its Friedel-like part and fluctuating part

\[ \mathcal{A} |\psi_i(r)|^2 = \frac{1}{\left(1 \pm \frac{\mathcal{L}}{2k_F\mathcal{A}}\right)} \left[1 \pm J_0(2k_Fx)\right] + \mathcal{A} \delta |\psi_i(r)|^2 \]

With a little algebra, one finds quickly that

\[ \langle S_i \rangle = i + \frac{i}{\mathcal{A}} \int_0^\infty dr \ \frac{J_1(2k_Fx)}{k_Fx} J_0(2k_Fx) = i \left(1 + \frac{2\mathcal{L}}{\pi k_F\mathcal{A}}\right) \]

To this first order correction, the average behavior is universal in that it neither depends on the nature of the dynamics nor on whether the boundary conditions are Dirichlet or Neumann.
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Normalization
Averages
Fluctuations

(a) $S_i - \langle S_i \rangle$

(cardioid billiard)

(b) $S_i - \langle S_i \rangle$

(stadium billiard)
Interest is in the leading order behavior of the variance
\[ \text{Var}[S_i - S_j] = \text{Var}[S_i] + \text{Var}[S_j] + \text{Covar}[S_i S_j] \]
as a function of \( k_F L \)

Skipping the gory details, the random plane wave model assumes that \( \text{Covar}[S_i S_j] = 0 \) and the calculations for fully chaotic systems give

\[ \text{Var}[S_i] = \text{Var}[S_j] = \frac{k_F L}{4\pi^3} \left\{ \begin{array}{ll}
2 \ln 2 - 1 \\
2 \ln 2 - 1 + 4 \ln \frac{\pi k_F A}{2L}
\end{array} \right. \]

Dirichlet b.c. Neumann b.c.

* for \( i = 1000 \), Neumann gives a result enhanced by approximately a factor 40 as compared to Dirichlet

** \( k_F L \) is \( O(i^{1/2}) \), i.e. the “i” scalings are \( i^{1/2} \) and \( i^{1/2} \ln i \)
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(a) \( \text{Var}[S_i] \)

\begin{align*}
0 & \quad 500 & \quad 1000 & \quad 1500 & \quad 2000 \\
0 & \quad \quad & \quad & \quad & \\
0 & \quad \quad & \quad & \quad & \\
0 & \quad \quad & \quad & \quad & \\
0 & \quad \quad & \quad & \quad & \\
1 & \quad \quad & \quad & \quad & \\
1 & \quad \quad & \quad & \quad & \\
2 & \quad \quad & \quad & \quad & \\
2 & \quad \quad & \quad & \quad & \\
3 & \quad \quad & \quad & \quad & \\
3 & \quad \quad & \quad & \quad & \\
\end{align*}

(cardioid billiard)

(b) \( \text{Var}[S_i] \)

\begin{align*}
0 & \quad 500 & \quad 1000 & \quad 1500 & \quad 2000 \\
0 & \quad \quad & \quad & \quad & \\
0 & \quad \quad & \quad & \quad & \\
0 & \quad \quad & \quad & \quad & \\
0 & \quad \quad & \quad & \quad & \\
200 & \quad \quad & \quad & \quad & \\
400 & \quad \quad & \quad & \quad & \\
600 & \quad \quad & \quad & \quad & \\
\end{align*}

(stadium billiard)

non-local statistical measures
Should random plane waves work?

Random waves

Stadium eigenstate
Semiclassical preliminaries

Generally speaking, semiclassical theory of chaotic systems necessitates energy smoothing, i.e.

\[ \overline{S}_{\Delta N} \overset{\text{def}}{=} \frac{1}{\Delta N} \sum_{E - \frac{\Delta E}{2} < E_i < E + \frac{\Delta E}{2}} S_i \]

One can extract individual state properties from the \( \Delta N \)-scaling because the variance is, in this notation

\[ \text{Var}[\overline{S}_{\Delta N}] \overset{\text{def}}{=} \left\langle \left( \overline{S}_{\Delta N} - \langle S \rangle \right)^2 \right\rangle = \frac{1}{\Delta N} \text{Var}[S_i] + \frac{\Delta N - 1}{\Delta N} \text{Covar}_{i \neq j}[S_i S_j] \]
In Bogomolny’s classic paper (Physica D, 1988), an extremely useful semiclassical approximation for the retarded Green function is given, which is needed here.

However, one has to be very careful making use of his expression, i.e. one must

- separate out the extremely short orbits responsible for the Friedel-like oscillations near the boundary
- keep the first correction terms to a density of states factor

His expression then takes the form

\[ \mathcal{A} |\overline{\Psi_i(r)}|^2_{\Delta N} = 1 \pm J_0(2k_F x) - \frac{1}{\pi \nu_W} \text{Im} \left( \tilde{G}_{\text{osc}}(r, r, E) \right)_{\Delta E} - \frac{1 \pm J_0(2k_F x)}{\mathcal{A} \nu_W} \rho_{\text{osc}}(E)_{\Delta E} \]
Chaotic quantum billiards

- From the Bogomolny expression, $S_i$ naturally decomposes into 3 components:
  - a short orbit Friedel-like part
  - the fluctuations of interest and “spurious” terms
  - density of states fluctuations that preserve norm and $\Delta N$, which are needed to cancel the otherwise spurious terms.

\[
S_i = \overline{S} \pm \left[ S_{i,osc}^{(1)} + S_{i,osc}^{(2)} \right]
\]

- The $\delta N(r,E)$ fluctuation terms are not kept as they are of lower order
- The short orbit term can be taken out of local energy averages
- A cluster of 4 orbits emerges for each contribution from stationary phase conditions properly applied
The bottom line is that a mean square of an angle function is replaced by its variance and doubled, thus

\[
\text{Var}(S_i) = \frac{k_F \mathcal{L}}{2\pi^3} \left\{ (2 \ln 2 - 1) - \left( \frac{\pi}{2} - 1 \right)^2 \\
(2 \ln 2 - 1) - \left( \frac{\pi}{2} - 1 \right)^2 + 4 \left( \ln \frac{\pi k_F A}{2 \mathcal{L}} - \frac{\pi}{2} \right) \right\}
\]
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(a) \text{Var}[S_i]

cardioid billiard

(b) \text{Var}[S_i]

stadium billiard

non-local statistical measures
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(a)

\[ \mathcal{F}_{\text{dos}}(L) \]

(b)

\[ \mathcal{F}(L) \]

non-local statistical measures
Deficiencies of random plane waves

1. Individual eigenstate normalization vs ensemble average normalization
   - directly leads to the replacement of the mean square by the variance

2. Improper dynamical correlations
   - After invoking the Hannay-Ozorio sum rule in the semiclassical theory, leads to factor two difference
For integrable systems, it is possible to give results based on an EBK-quantized tori approach

To give an example, consider the circular billiard (note the $i$-dependence)

$$\text{Var}[S_i] = i \times \left\{ \frac{2}{\pi} - \frac{1}{2} - \left(1 - \frac{2}{\pi}\right)^2 \approx 0.00457 \quad \text{Dirichlet} \right. $$

$$\left. - \frac{2}{\pi} - \frac{1}{2} + \pi^{1/2}i^{1/4} - \left(1 - \frac{2}{\pi}\right)^2 \quad \text{Neumann} \right\}$$

It is possible using a modification of rectangle eigenstates to derive an expression for the influence of the bouncing ball modes (we rely on Tanner’s estimate (J. Phys. A, 1997) of the relative fraction of bouncing ball modes), but the expression is too long and cumbersome to write on a slide... though shown on the variance figure
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Ultra-cold Fermi gasses provide other quantities in the same category as the \( \{S_i\} \), e.g. BCS pairing gap fluctuations [see Garcia-Garcia et al. PRL, 2008 and Olofsson et al. PRL, 2008].