Long-range energy-level interaction in small metallic particles

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We consider the energy level statistics of non-interacting electrons which diffuse in a d-dimensional disordered metallic conductor of characteristic Thouless energy $E_c$. We assume that the level distribution can be written as the Gibbs distribution of a classical one-dimensional gas of fictitious particles with a pairwise additive interaction potential $f(\varepsilon)$. We show that the interaction which is consistent with the known correlation function of pairs of energy levels is a logarithmic repulsion for level separations $\varepsilon < E_c$, in agreement with Random Matrix Theory. When $\varepsilon > E_c$, $f(\varepsilon)$ vanishes as a power law in $\varepsilon/E_c$ with exponents $-\frac{1}{2}, -2$, and $-\frac{3}{2}$ for $d = 1, 2, 3$, respectively. While for $d = 1, 2$ the energy-level interaction is always repulsive, in three dimensions there is long-range level attraction after the short-range logarithmic repulsion.

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A statistical description of the Hamiltonian $H$ of a complex system is provided by random matrix theory. A key feature in this theory is the spectral rigidity of the energy levels: their distribution $P(E_1, E_2, \ldots E_N)$ formally coincides with the Gibbs distribution of the positions of a one-dimensional gas of $N$ classical particles with a repulsive logarithmic interaction,

$$ P(\{E_n\}) = Z^{-1} \exp\left[ -\beta \mathcal{H}(\{E_n\}) \right], \quad (1) $$

$$ \mathcal{H}(\{E_n\}) = - \sum_{i<j} \ln |E_i - E_j| + \sum_i V(E_i). \quad (2) $$

Here $Z$ is a normalization constant, and $V(E)$ is a confining potential. The parameter $\beta$, playing the role of an inverse temperature, depends on the symmetry class of the ensemble of random Hamiltonians $H$. A method which yields such a distribution consists in assigning to the Hamiltonian $H$ a probability distribution of maximum information entropy given a spectral constraint $\mathcal{H}$. For instance, a constraint on the expectation value of $\sum_i E_i^2$ yields the Gaussian ensembles, where $V(E) \propto E^2$. Other ensembles, characterized by different $V(E)$, result from other spectral constraints (e.g. the averaged level density). All these classical ensembles of random matrices have in common an absence of eigenvalue–eigenvector correlations and a logarithmic repulsion between pairs of eigenvalues.

The use of this theory for the study of electronic properties of small metallic particles was introduced by Gorkov and Eliashberg. Theoretical support for the logarithmic repulsion of energy levels came with the work of Efetov. Assuming bulk diffusion of the electrons by elastic scatterers and using a supersymmetric formalism, he obtained for the spectrum of small metallic particles the same correlation function as in classical sets of random matrices. Subsequently, addressing the connection between universal conductance fluctuations and the universal properties of random matrices, Al’ishuler and Shklovskii (A&S) showed that for energy separations $|E - E'| > E_c$ the correlation function deviates from classical random matrix theory. The Thouless energy $E_c = \text{Dh}/L^2$ is inversely proportional to the time $\tau_{\text{erg}}$ it takes an electron to diffuse (with diffusion coefficient $\text{D}$) across a particle of size $L$. The results of the diagrammatic perturbation theory of A&S were recently rederived by Argaman, Imry, and Smilansky, using a more intuitive semiclassical method.

One would not expect that the logarithmic level repulsion in Eq. (2) holds for levels which are separated by more than $E_c$. What is then the long-range energy-level interaction in small metallic particles? This is the question addressed in this paper. In a sense, this is an inverse problem in statistical mechanics: given the pair correlation function, what is the interaction potential? Our analysis applies a recently developed functional-derivative technique to compute correlation functions in random-matrix ensembles with an arbitrary two-body interaction potential. The restriction to two-body (i.e. pairwise additive) interaction is our single assumption. We find that $E_c$ characterizes a cross-over between a short-range logarithmic repulsion and a novel long-range part which decays as a power law, with a dimensionality-dependent exponent. The interaction remains repulsive for dimensions 1 and 2, but exhibits a long-range attractive part after a short-range repulsion in 3 dimensions.

The starting point of our analysis is the Gibbs distribution (1) with an arbitrary two-body interaction $f(|E - E'|)$ in the fictitious “Hamiltonian” $\mathcal{H}$,

$$ \mathcal{H}(\{E_n\}) = \sum_{i<j} f(|E_i - E_j|) + \sum_i V(E_i). \quad (3) $$

The mean eigenvalue density $\langle \rho(E) \rangle = \langle \sum_n \delta(E - E_n) \rangle$ (where $\langle \ldots \rangle$ denotes an average with weight $P(\{E_n\})$)
is related to $V(E)$ and $f(E - E')$ by an integral equation, valid\textsuperscript{[9]} to the leading order of a $1/N$ expansion:

$$V(E) = -\int_{-\infty}^{\infty} dE' \langle \rho(E') \rangle f(|E - E'|) + c . \tag{4}$$

The constant $c$ is to be determined from the normalization condition $\int dE \langle \rho(E) \rangle = N$. Eq. (4) has the intuitive “mean-field” interpretation (originally due to Wigner), that the “charge density” $\langle \rho \rangle$ adjusts itself to the “external potential” $V$ in such a way that the total force on any charge $E$ vanishes. Dyson\textsuperscript{[9]} has evaluated the first correction to Eq. (4), which is smaller by a factor $N^{-1}$ in $N$.

The density-density correlation function defined by

$$K_2(E, E') = \langle \rho(E) \rangle \langle \rho(E') \rangle - \langle \rho(E) \rangle \langle \rho(E') \rangle , \tag{5}$$

can be expressed as a functional derivative\textsuperscript{[8]},

$$K_2(E, E') = \frac{1}{\beta} \frac{\delta \langle \rho(E) \rangle}{\delta V(E')} . \tag{6}$$

Eq. (6) is an exact consequence of Eqs. (1) and [3]. Physically, it means that correlations between $E$ and $E'$ are important when a modification of the potential at $E'$ has a substantial impact on the mean density at $E$. Combining Eqs. (4) and (6), one can see that $K_2(E, E') \equiv K_2(|E - E'|)$ is translationally invariant and independent of the confining potential $V(E)$, depending on the two-body interaction $f(\varepsilon)$ only. This property is at the heart of universality in random-matrix theory\textsuperscript{[8][9]}.

By Fourier transforming the convolution (4), the time-dependent two-body form factor

$$K_2(t) = \int_{-\infty}^{\infty} d\varepsilon K_2(\varepsilon) \exp \left( -\frac{i\varepsilon t}{\hbar} \right) \tag{7}$$

can be written as

$$K_2(t) = \frac{1}{\beta f(t)} \delta \langle \rho(t) \rangle = -\frac{1}{\beta f(t)} . \tag{8}$$

This relationship gives us the prescription for obtaining the eigenvalue interaction $f(\varepsilon)$ from the density-density correlation function $K_2(\varepsilon)$.

For disordered systems in the weak-scattering limit, A&K\textsuperscript{[S]} have shown by perturbation theory that the correlation function is given by

$$K_2(\varepsilon) = \frac{s^2}{\beta \pi^2} \text{Re} \sum_{\{n_\mu\}} (\varepsilon + i\hbar Dq^2 + i\gamma)^{-2} , \tag{9}$$

for energies $\varepsilon$ large compared to the level spacing $\Delta$, and small compared with the energy scale $\hbar/\tau_e$, associated with the elastic scattering time $\tau_e$. The factor $s = 2$ accounts for the spin degeneracy of each level, $\gamma$ is a small energy cutoff (to account for inelastic scattering) and the parameter $\beta$ equals $1$ (2) in the presence (absence) of time-reversal symmetry ($\beta = 4$ for time-reversal symmetry with strong spin-orbit scattering). The sum is over the eigenvalues of the diffusion equation for the sample, assumed to be a $d$-dimensional parallelepiped with sides $L_\mu$ ($q^2 = \pi^2 \sum_{\mu=1}^{d} (n_\mu/L_\mu)^2$). In what follows we put $s = 1$ and $\gamma = 0$, ignoring the spin degeneracy and the small-energy cutoff. The Fourier transform of Eq. (9) is

$$K_2(t) = -\frac{|t|}{\beta \pi \hbar} \sum_{\{n_\mu\}} \exp \left( -D\pi^2 |t| \sum_{\mu=1}^{d} (n_\mu/L_\mu)^2 \right) . \tag{10}$$

The long- and short-range limits $K_2^1(t)$ and $K_2^2(t)$ of the form factor (10) can be obtained in closed form\textsuperscript{[7]}. The cross-over time scale is the so called ergodic time $t_{\text{erg}} = L^2/D$, which it takes an electron to explore the whole available phase space (for simplicity we work with a hypercube, $L_\mu = L$ for all $\mu$). The ergodic time is related to the Thouless energy by $E_{\text{Th}} = \hbar/t_{\text{erg}}$. For times $t \gg t_{\text{erg}}$ the first term of Eq. (10) dominates the sum, while for $t \ll t_{\text{erg}}$ one can convert the sums over $n_\mu$ into gaussian integrals. The resulting long- and short-time limits are\textsuperscript{[7]}:

$$K_2^1(t) = -\frac{|t|}{\beta \pi \hbar} , \tag{11}$$

$$K_2^2(t) = -\frac{|t|}{\beta \pi \hbar} \left( 4\pi D \right)^{d/2} . \tag{12}$$

For analytical work it is convenient to have an expression which smoothly interpolates between these two asymptotic limits. We will use the interpolation formula

$$K_2(t) \approx K_2^1(t) + K_2^2(t) . \tag{13}$$

The approximation (13) differs from the full expression (10) for $t \approx t_{\text{erg}}$, but it is accurate for $t$ either much smaller or much larger than $t_{\text{erg}}$. This is sufficient for the purpose of obtaining the asymptotic behavior of the interaction potential.

Combining Eqs. (6) and (13), the interaction potential $f_d(\varepsilon)$ for $d$ dimensions can be written as

$$f_d(\varepsilon) = \int_{0}^{\infty} dt \ \cos(\alpha t) \frac{t^{d/2}}{t(1 + t^{d/2})} , \tag{14}$$

where $\alpha = \varepsilon/(4\pi E_v)$ is the dimensionless energy variable. The integral (14) can be evaluated numerically for all $\alpha$, and analytically in the small- and large-$\alpha$ limits. For $|\alpha| \ll 1$ we can approximate $\cos \alpha t \simeq 1$ and cut the upper integration limit at $1/|\alpha|$, which readily yields the short range universal logarithmic interaction $f_d(\varepsilon) \simeq -\ln|\alpha|$. For $|\alpha| \rightarrow \infty$ the high-frequency oscillations of $\cos \alpha t$
average the integral to zero, in a way which depends on the dimensionality. The easiest case is \( d = 2 \), where the integral can be evaluated in a closed form,

\[
f_{2}(\varepsilon) = -\sin |\alpha| \sin |\alpha| - \cos (\alpha) \cos (\alpha),
\]

which behaves as \(-\ln |\alpha| - C\) for small \(|\alpha|\) (\(C\) is Euler’s constant), and \(1/\alpha^2\) is the dominant term of an asymptotic expansion of Eq. (14) for \(|\alpha| \gg 1\). We therefore recover the short-range logarithmic repulsion and find that the interaction remains repulsive in the whole energy range. For \( d = 3 \), the asymptotic limits of the interaction can be obtained by considering the auxiliary function

\[
h(\alpha) = \int_{0}^{\infty} dt \frac{\sin \alpha t}{t} \frac{t^{1/2}}{1 + t^{3/2}},
\]

which satisfies \(h'(\alpha) = f_{3}(\alpha)\) as well as the differential equation

\[
h'(\alpha) = \frac{1}{\alpha} h(\alpha) - \frac{3}{\alpha} \int_{0}^{\infty} du \sin (\alpha u^2) \left( 1 + u^2 \right) \frac{1}{\left( 1 + u^2 \right)^{3/2}}.
\]

The second term on the r.h.s. becomes \(-1\) in the small-\(\alpha\) limit, and \(-3\sqrt{\pi}|2\alpha|^{-3/2}\) in the large-\(\alpha\) limit. We thus obtain \(f_{3}(\varepsilon) \approx -\ln |\alpha| - C\) for \(|\alpha| \ll 1\) and \(-\sqrt{|2\alpha|}^{-3/2}\) for \(|\alpha| \gg 1\). Therefore, in \( d = 3 \), we have an attractive eigenvalue interaction for large separations. Using a similar procedure for \( d = 1 \) we obtain the same short-range logarithmic repulsion \(-\ln |\alpha| - C\), which crosses over to an algebraic repulsion \(f_{1}(\varepsilon) \simeq \sqrt{\pi}|2\alpha|^{-1/2}\) for \(|\alpha| \gg 1\).

In Fig. 1 we compare a numerical integration of Eq. (14) with the asymptotic expressions derived above, which we summarize:

\[
f_{d}(\varepsilon) = -\ln \left| \frac{\varepsilon}{4\pi E_{c}} \right| - C \quad \text{if } |\varepsilon| \ll E_{c},
\]

\[
f_{1}(\varepsilon) = \left( \frac{\varepsilon}{4\pi E_{c}} \right)^{1/2} \left| \frac{\varepsilon}{4\pi E_{c}} \right|^{-1/2} \quad \text{if } |\varepsilon| \gg E_{c},
\]

\[
f_{2}(\varepsilon) = \left( \frac{\varepsilon}{4\pi E_{c}} \right)^{1/2} \left| \frac{\varepsilon}{4\pi E_{c}} \right|^{-3/2} \quad \text{if } |\varepsilon| \gg E_{c},
\]

\[
f_{3}(\varepsilon) = -\frac{1}{2} \left( \frac{\varepsilon}{4\pi E_{c}} \right)^{1/2} \left| \frac{\varepsilon}{4\pi E_{c}} \right|^{-3/2} \quad \text{if } |\varepsilon| \gg E_{c}.
\]

Fig. 1 shows the crossover from the universal logarithmic short-range repulsion into the novel long-range power-law regime (repulsive for \( d = 1,2 \) and attractive for \( d = 3 \)).

In summary, we have calculated in the metallic regime the dimensionality–dependent long-range part of the energy-level interaction. From this interaction, one could in principal calculate \(n\)-point correlation functions for arbitrary \(n\). Our method is based on a general relation [8] between the density-density correlation function and this interaction. We use it in a particular case where this correlation function is known from diagrammatic perturbation theory [9] (or an equivalent semiclassical theory [7]). The validity of our results is restricted to the validity of these perturbative or semiclassical approaches: \(\varepsilon \gg \Delta\), and \(\varepsilon \ll h/\tau_{c}\). Since Efetov has shown that random matrix theory remains valid for \(\varepsilon \ll \Delta\), the universal logarithmic repulsion which we recover must be also valid for these small energy separations, though either perturbation theory (Eq. (9)), or our method based on an asymptotic large-N approximation misses fine structure on the scale of \(\Delta\).

The condition \(\varepsilon \ll h/\tau_{c}\) limits the non-universal algebraic decay which we find for \(\varepsilon > E_{c} \equiv h/\tau_{erg}\). These non-universal interactions result from the non-ergodic electron dynamics for \(t < t_{erg}\). The non-ergodic dynamics in our problem is unbounded diffusion in \(d\) dimensions. For times smaller than \(\tau_{c}\) the electron motion is ballistic, a behaviour which is not considered in our theory.

Chaotic billiards with ballistic motion between the boundaries constitute another example for the applicability of random-matrix theory. In the semiclassical limit the energy level correlations are also correctly described by the classical ensembles for energy differences smaller than the inverse period of the shortest periodic orbits of the system [10] [11]. The essential difference with the small metallic particles considered in this work is that these have a well-defined statistical regime of diffusive motion between \(\tau_{c}\) and \(t_{erg}\).

It is interesting to consider the scale dependence of the interaction potential. In \( d = 3 \), the level spacing scales as \(\Delta \propto L^{-3}\) while \(E_{c} \propto L^{-2}\), so that \(\Delta \ll E_{c}\) as \(L \rightarrow \infty\). Therefore, if we measure \(|E - E'|\) in units of \(\Delta\), the interaction \(f(E - E')\) scales with \(L\) towards the

![Fig. 1: Interaction potential according to Eq. (14) for various spatial dimensions \(d\) (solid), together with the short-range logarithmic (dash) and long-range power law (dot-dash) asymptotic forms described by Eqs. (15) and (19). Inset: blow up of the departure from the short-range logarithmic interaction.](image-url)
universal random matrix repulsion for about $L$ nearest neighbour levels for three dimensional conductors. However, the total number of levels being proportional to $L^3$, the relation (4) between the average density $\langle \rho(E) \rangle$ and the confining potential $V(E)$ still differs from the usual expression (i.e. with a logarithmic interaction) in the thermodynamic limit.

Our analysis is restricted to metallic particles which are small compared with the localization length. In the thermodynamic limit, electrons are always localized for $d = 1$ or 2 (except for $\beta = 4$ in $d = 2$ at low disorder). Anderson localization occurs also in three dimensions for large disorder. In these cases, our perturbative starting point Eq. (9) is no longer valid. In the presence of eigenvector localization, $f(\varepsilon)$ probably scales with the system size towards a delta function (uncorrelated levels in the limit of strong localization). An interesting issue that we postpone for future studies is to see if the mobility edge is characterized by some scale invariant interaction $f_c(\varepsilon)$.

In this paper we have only considered the eigenvalue statistics. The classical random matrix ensembles are invariant under canonical (orthogonal, unitary or symplectic) transformations. The logarithmic level repulsion is related to the maximum randomness of the eigenvectors. In the localized regime, it is clear that the absence of a logarithmic level repulsion has its physical origin in the localization of the eigenvectors in different parts of the system. An important issue would consists in identifying what kind of modification of the eigenvector statistics from Porter-Thomas distribution [1] is behind the novel non-universal part of the level interaction found in this work.

Finally, it is likely that studies similar to the one presented here for the hamiltonian ensemble will be useful for the ensemble of scattering or transfer matrices [12], and will improve our understanding of quantum transport in disordered conductors.

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