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Long-Range Energy Level Interaction in Small Metallic Particles.

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Abstract. – 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 the random matrix theory. When $\varepsilon > E_c$, $f(\varepsilon)$ vanishes as a power law in ε/E_c with exponents $-1/2$, -2, and $-3/2$ for $d = 1$, 2, and 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.

A statistical description of the Hamiltonian $\boldsymbol{H}$ of a complex system is provided by the 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 on N classical particles with a *repulsive logarithmic interaction*,

$$P(\{E_n\}) = Z^{-1} \exp[-\beta \mathscr{H}(\{E_n\})], \tag{1}$$

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

Here Z is a normalization constant, and $V(E)$ is a confining potential. The parameter β, playing the role of an inverse temperature, depends on the symmetry class of the ensemble of random Hamiltonians [1]. A method which yields such a distribution consists in assigning to the Hamiltonian $\boldsymbol{H}$ a probability distribution of maximum information entropy given a spectral constraint [2]. 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 the 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 [3]. Theoretical support for the logarithmic repulsion of energy levels came with the work of Efetov [4]. Assuming bulk diffusion of the electrons by elastic scatterers, he obtained for the spectrum of metallic particles the same correlation function as in classical sets of random matrices. Subsequently, addressing the connection between universal conductance fluctuations [5] and the universal properties of random matrices, Al'tshuler and Shklovskiĭ [6] showed that, for energy separations $|E - E'|$ greater than the Thouless energy E_c, the correlation function deviates from the classical random matrix theory. The relevant crossover energy scale $E_c = D\hbar/L^2$ is inversely proportional to the time t_{erg} it takes for an electron to diffuse (with diffusion coefficient D) across a particle of size L. The results of the perturbation theory were recently rederived by Argaman, Imry, and Smilansky, using a more intuitive semi-classical method [7].

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? To address this question, we use a recently developed functional-derivative technique to compute correlation functions in random matrix ensembles with an arbitrary two-body interaction potential [8]. The restriction to two-body (*i.e.* pairwise additive) interaction is our single assumption. We find that E_c characterizes a crossover 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» $\mathscr{H}$,

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

The mean eigenvalue density $\langle\rho(E)\rangle$ is related to $V(E)$ and $f(E - E')$ by an integral equation, valid [9] to the leading order of a $1/N$ expansion:

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

Equation (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 [9] has evaluated the first correction to eq. (4), which is smaller by a factor $N^{-1}\ln N$.

The density-density correlation function defined by

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

can be expressed as a functional derivative [8],

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

Equation (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 the random matrix theory [8, 9].

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

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

can be written as

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

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, the perturbation theory gives [6]

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

for energies ε large compared to the level spacing Δ, and small compared with the energy scale $\hbar/\tau_e$, associated with the elastic-scattering time τ_e. The factor $s = 2$ accounts for the spin degeneracy of each level, γ is a small-energy cut-off (to account for inelastic scattering) and the parameter β 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 $L_\mu\left(q^2 = \pi^2\sum_{\mu=1}^{d}(n_\mu/L_\mu)^2\right)$. In what follows we put $s = 1$ and $\gamma = 0$, ignoring the spin degeneracy and the small-energy cut-off, and we work for simplicity with a hypercube of size L. The Fourier transform of eq. (9) is

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

The long- and short-range limits $K_2^{\mathrm{l}}(t)$ and $K_2^{\mathrm{s}}(t)$ of the form factor (10) can be obtained in closed form [7]. The crossover time scale is the ergodic time $t_{\mathrm{erg}} = \hbar/E_c$. For times $t \gg t_{\mathrm{erg}}$ the first term of eq. (10) dominates the sum, while for $t \ll t_{\mathrm{erg}}$ one can convert the sums over n_μ into Gaussian integrals. The resulting long- and short-time limits are [7]

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

$$K_2^{\mathrm{s}}(t) = -\frac{|t|}{\beta\pi\hbar}\frac{L^d|t|^{-d/2}}{(4\pi D)^{d/2}}\,. \tag{11b}$$

We use the interpolation formula

$$K_2(t) \simeq K_2^{\mathrm{l}}(t) + K_2^{\mathrm{s}}(t)\,, \tag{12}$$

which is sufficient for the purpose of obtaining the asymptotic behaviour of the interaction potential.

Combining eqs. (6) and (12), the interaction potential $f_d(\varepsilon)$ for d dimensions can be written as

$$f_d(\varepsilon) = \int_0^{\infty}\mathrm{d}t\cos(\alpha t)\frac{t^{d/2}}{t(1+t^{d/2})}\,, \tag{13}$$

where $\alpha = \varepsilon/(4\pi E_c)$ is the dimensionless energy variable. The integral (13) can be evaluated numerically for all α, and analytically in the small- and large-α 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 $|\alpha| \to \infty$ 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,

$$f_2(\varepsilon) = -\sin|\alpha|\,\mathrm{si}\,|\alpha| - \cos(\alpha)\,\mathrm{ci}(\alpha)\,, \tag{14}$$

which behaves as $-\ln|\alpha| - \mathcal{C}$ for small $|\alpha|$ ($\mathcal{C}$ is Euler's constant), and $1/\alpha^2$ is the dominant term of an asymptotic expansion of eq. (13) 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

$$h(\alpha) = \int_0^\infty \mathrm{d}t \frac{\sin \alpha t}{t} \frac{t^{1/2}}{1 + t^{3/2}}\,, \tag{15}$$

which satisfies $h'(\alpha) = f_3(\alpha)$ as well as the differential equation

$$h'(\alpha) = \frac{1}{\alpha} h(\alpha) - \frac{3}{\alpha} \int_0^\infty \mathrm{d}u \frac{\sin(\alpha u^2)}{(1 + u^3)^2}\,. \tag{16}$$

The second term on the r.h.s. becomes -1 in the small-α limit, and $-3\sqrt{\pi}|2\alpha|^{-3/2}$ in the large-α limit. We thus obtain $f_3(\varepsilon) \simeq -\ln|\alpha| - \mathcal{C}$ for $|\alpha| \ll 1$ and $-\sqrt{\pi}|2\alpha|^{-3/2}$ 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 $-\ln|\alpha| - \mathcal{C}$, 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. (13) with the asymptotic expressions derived above, which we summarize:

$$f_d(\varepsilon) = -\ln\left|\frac{\varepsilon}{4\pi E_c}\right| - \mathcal{C} \qquad \text{if } |\varepsilon| \ll E_c\,, \tag{17a}$$

$$\left.\begin{aligned} f_1(\varepsilon) &= \left(\frac{\pi}{2}\right)^{1/2}\left|\frac{\varepsilon}{4\pi E_c}\right|^{-1/2} \\ f_2(\varepsilon) &= \left(\frac{\varepsilon}{4\pi E_c}\right)^{-2} \\ f_3(\varepsilon) &= -\frac{1}{2}\left(\frac{\pi}{2}\right)^{1/2}\left|\frac{\varepsilon}{4\pi E_c}\right|^{-3/2} \end{aligned}\right\} \quad \text{if } |\varepsilon| \gg E_c\,. \tag{17b}$$

Figure 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 $d = 3$).

We have used microscopic theories for having $K_2(\varepsilon)$. The validity of our results is then restricted to the validity of these perturbative or semi-classical approaches: $\varepsilon \gg \Delta$, and $\varepsilon \ll \hbar/\tau_e$. Since Efetov has shown that the 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 miss fine structure on the scale of Δ.

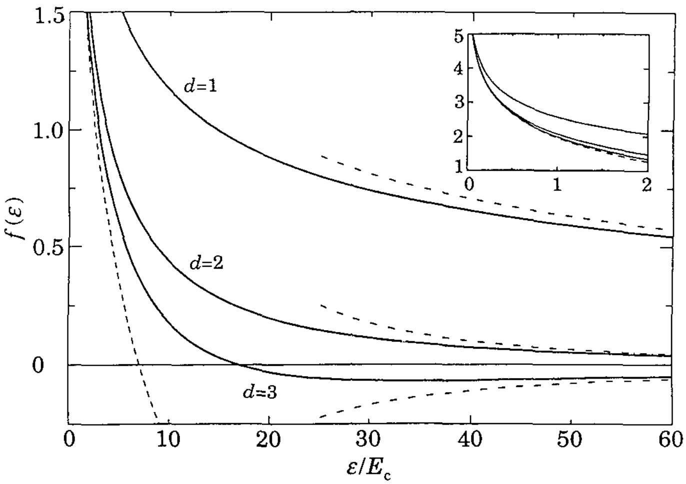

Fig. 1. – Interaction potential according to eq. (13) for various spatial dimensions d (solid line), together with the short-range logarithmic (dashed line) and long-range power law (dot-dashed line) asymptotic forms described by eqs. (17). Inset: blow-up of the departure from the short-range logarithmic interaction.

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

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 $L \to \infty$. Therefore if we measure $|E - E'|$ in units of Δ, the interaction $f(E - E')$ scales with L towards the 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 equation (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 determine the scale-invariant behaviour $f_c(\varepsilon)$ of the interaction at the mobility edge. Such a behaviour can be conjectured from a recent numerical study [10] showing that the level spacing distribution is scale invariant at the mobility edge.

In summary, we have calculated in the metallic regime the dimensionality-dependent long-range part of the energy level interaction. We have found in three dimensions a completely unexpected crossover from level repulsion to level attraction. 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 perturbation theory (or an equivalent semi-classical theory). Our single basic assumption is that the full many-body interaction of the energy levels is an arbitrary two-body interaction.

If this is exact, $f(\varepsilon)$ bears the complete information about the spectral statistics, and our result provides a generating functional formalism for the calculations of all n-level correlation functions. However, the known methods of integration of eq. (1), using orthogonal polynomials, cannot be used with our new $f(|\varepsilon|)$. This makes the calculation of high-order correlations difficult. The n-order cumulants of the density of states, evaluated at the same energy only, are given by Al'tshuler, Kravtsov and Lerner (see ref. [5]) from a field-theoretical representation for the moments of mesoscopic fluctuations. An interesting issue would consist in obtaining from our new interaction the slow logarithmically normal decay of the probability of very large fluctuations.

However, even if our basic assumption turns out not to give the same n-level correlation as the microscopic models, our result would still show what the level interaction becomes, when treated as an effective «self-consistent» two-body interaction. This opens up a new problem in the random matrix theory, to identify what kind of modification of the eigenvector statistics from Porter-Thomas distribution [1] generates the correct long-range behaviour of the correlation function obtained by microscopic theory. The classical random matrix ensembles are invariant under canonical (orthogonal, unitary or symplectic) transformations and the infinite-range logarithmic-level repulsion results from the maximum randomness of the eigenvectors, in a maximum-entropy approach. In the limit of strong disorder (localized regime), when the kinetic energy is negligible compared to the strength of the random fluctuations of the electrostatic potential, a more natural basis, where the Hamiltonian is likely to be almost diagonal, is given by appropriate local-site wave functions. This is why in this limit the range of the logarithmic interaction must shrink to smaller and smaller intervals. Our result indicates that even for weaker disorder (metallic regime) $\boldsymbol{H}$ cannot be statistically invariant under change of basis and that a new constraint (ignored thus far) on the eigenvectors is required to describe level separation larger than E_c.

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