Fast Ground-State Reordering from Off-Diagonal Fluctuations of Interaction

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(November 8, 2018)

It is shown that off-diagonal fluctuations of interaction lead to the breakdown of perturbation theory in the immediate vicinity of the ground-state of a fermionic system at a rate inversely proportional to the number of considered particles. This rate is parametrically much faster than previously expected. It is shown that this follows from the coherent addition of many small second order contributions to the energy of low-lying levels.

PACS numbers: 73.23.-b, 71.10.-w, 71.24.+q, 75.10.Lp

Random interactions naturally occur in various fields of physics. Assuming the symmetry of the probability distribution of the one-body Hamiltonian under unitary basis transformation in Hilbert space directly results in the randomness and a similar symmetry for the distribution of the Interaction Matrix Elements (IME). Typically, this symmetry is satisfied up to an energy scale $E_c$ (the Thouless energy) so that models with random interactions may be expected to describe interacting systems provided one restricts oneself to energy scales of an order of magnitude given by $E_c$. In condensed-matter systems, this corresponds to one-body excitation energies inside a window of width $E_c = g \Delta$ around the Fermi energy, hence containing a finite number of levels given by the conductance $g$ ($\Delta$ is the mean level spacing).

Random Interaction Models (RIM) first appeared in nuclear physics and early investigations focused on the deviations from Random Matrix Theory introduced by nuclear shell model calculations \cite{1}. The complexity of the excited spectrum of rare-earth atoms motivated the introduction of RIM in atomic physics \cite{2}, and RIM reproduced statistical features obtained in nuclear shell model calculations \cite{3}. Last but not least, RIM were used in condensed matter physics to study the quasiparticle lifetime \cite{4} and the conductance peak spacings and heights distributions \cite{5} in quantum dots in the Coulomb blockade regime. More recently a lot of attention has been devoted to the properties of the ground-state of RIM \cite{6, 7} and several spectral features presented in these latter investigations indicate that RIM are realistic down to very low excitation energies. It is the purpose of the present letter to investigate in detail the ground-state structure of systems of few ($n$) fermions as the relative strength $U/\Delta$ of fluctuations of interaction increases. The main result of these investigations is a breakdown of perturbation theory for the ground-state at a critical value $U_c(n) \sim \Delta/n$. In particular, $U_c$ is parametrically smaller by a factor $1/n$ than previously suggested \cite{8}. Once this threshold is reached, the ground-state starts to be composed of an exponentially large number of Slater determinants, an occurrence which goes far beyond a simple renormalization of one-particle orbitals. We will see that this is due to the coherent addition of large numbers of small second order contributions for perturbation theory in the immediate vicinity of the ground-state.

We investigate a model for spin-1/2 fermions

$$H = \sum \epsilon_{c} c_{\alpha,s}^\dagger c_{\alpha,s} + \sum U_{\alpha,\beta}^{\gamma,\delta} c_{\alpha,s}^\dagger c_{\beta,s} c_{\gamma,s}^\dagger c_{\delta,s} \quad (1)$$

The greek indices label $m/2$ different one-body energies which are distributed as $\epsilon_{c} \in [0;m/2]$ so that the mean spacing between spin-degenerate levels is $\Delta \equiv 1$ and $s^{(c)} = \uparrow, \downarrow$ are spin indices. The Hamiltonian is Spin Rotational Symmetric (SRS): the interaction commutes with both the total spin $|\bar{S}|$ and its projection $S_z$. The corresponding eigenvalues $\sigma$ and $\sigma_z$ are good quantum numbers and the Hamiltonian matrix acquires a block structure where blocks are labelled by $\sigma_z$ and $\sigma$. From now on we consider only the $\sigma = \sigma_z = 0$ ($1/2$) block for $n$ even (odd). The results and arguments presented below can however be generalized to higher spin blocks or models of spinless fermions.

The Hamiltonian (1) can be viewed as a model of interacting fermions expressed in the basis of Slater determinants constructed from the set of one-particle eigenfunctions $\psi_{\alpha}$ of $H_0 \equiv \sum \epsilon_{c} c_{\alpha,s}^\dagger c_{\alpha,s}$. In this basis, the IME are given by $U_{\alpha,\beta}^{\gamma,\delta} = \sum_{i,j} U(i - j) \psi_{\alpha}^*(i) \psi_{\beta}^*(j) \psi_{\gamma}(i) \psi_{\delta}(j)$, where $U(i - j)$ is the interaction potential in real space; $i$ and $j$ label sites on a lattice. Assuming that the presence of disorder or chaotic boundary scattering confers a random character to the $\psi_{\alpha}$’s directly leads to fluctuations of the $U_{\alpha,\beta}^{\gamma,\delta}$ around their average value. Only diagonal matrix elements have a nonzero average leading to mean-field charge-charge, spin-spin and BCS interactions \cite{9} which we will neglect as they have at most a marginal influence on the object of interest here. We therefore take the IME in (1) to be randomly distributed inside a zero-centred Gaussian distribution of width $U$, $P(U_{\alpha,\beta}^{\gamma,\delta}) \propto e^{-(U_{\alpha,\beta}^{\gamma,\delta})^2/2U^2}$.

We start with a perturbative calculation of the ground-state energy up to the second order in the small parameter $U/\Delta \ll 1$. The first order correction vanishes on average, and the second order correction can be written
\[ \Delta \mathcal{E}_0^{(2)} = \sum \frac{(U_{\alpha}^\gamma \delta)^2}{\epsilon_{\gamma} + \epsilon_{\delta} - \epsilon_{\alpha} - \epsilon_{\beta}} \]  

\( \sum \) indicates that the sum is taken over occupied levels \( \gamma \) and \( \delta \) and unoccupied ones \( \alpha \) and \( \beta \) (taking into account spin degeneracy), giving a total number of contributions \( K \sim n^2(m-n)^2 \). For the ground-state, one has \( \epsilon_{\gamma} + \epsilon_{\delta} < \epsilon_{\alpha} + \epsilon_{\beta} \), and each term in the sum (2) is negative. The contributions from each scattering process therefore add coherently resulting in a strong reduction of the ground-state energy. The latter can be estimated for an equidistant spectrum by replacing sums by integrals in (2). This gives an homogeneous polynomial of order three in \( n \) and \( m \), each term being multiplied by a logarithmic correction. In the dilute limit \( 1 \ll n \ll m \) the \( n^3 \) and \( m^2 n \) terms drops out exactly so that the dominant contribution to the second order correction in the ground-state energy reads

\[ \Delta \mathcal{E}_0^{(2)} \approx -A(U^2/\Delta)n^2 m \log(m) \]  

(3)

The prefactor \( A \) can be estimated \( A \approx 7 \); details of the perturbative treatment are presented elsewhere [14].

In Fig.1 we show the behavior of the ground-state energy for \( n = 2, 4, 6 \) and 8. It is clearly seen that the average ground-state energy exhibits the quadratic dependence in \( U \) predicted by (2-3) at weak \( U \), while at larger \( U \), this dependence becomes linear. Most importantly, this crossover occurs at a weaker \( U \) for larger \( n \). Both these features can be understood as one realizes that for dominant fluctuations of interaction \( U/\Delta \gg 1 \) the Hamiltonian depends linearly in \( U \). In this regime, and for \( n \gg 1 \), the average many-body density of states is Gaussian with a width \( B \) well approximated by \( B \sim n m U \).

\[ \ref{[13,14]} \text{ This width thus gives a good parametric estimate for the average ground-state energy in the asymptotic regime } \Delta \mathcal{E}_0^{(2)} \sim B \sim n m U \] so that equating the asymptotic and perturbative expressions for the ground-state energy \( \Delta \mathcal{E}_0^{(2)} \sim n m U \) gives a critical value

\[ U_c \sim \Delta/n \]  

(4)

The crossover between the two regimes occurs at a rate given by \( U_c \) and is inversely proportional to the number of particles. As can be seen in Fig.1, below this threshold, the ground-state energy is well approximated by the second order perturbation expression (3), while above it, its \( U \)-dependence becomes linear which cannot be captured by any finite order of perturbation theory, and we are forced to conclude that \( U_c \) gives the radius of convergence for perturbation theory in \( U \).

For \( U > U_c \), the ground-state starts to be mixed with higher excited states and the number of Slater determinants \( |J| \) necessary to construct it becomes much larger than one. A measure of this number is given by the Participation Ratio (PR), which, for a given many-body eigenstate \( |\Psi_\lambda(U)\rangle \), is defined as \( \xi_\lambda = (\sum_j (|\langle J|\Psi_\lambda(U)\rangle|^2)^2/\sum_j (|\langle J|\Psi_\lambda(U)\rangle|^4)^4 \). If \( |\Psi_\lambda(U)\rangle \) is made up of one single Slater determinant (as it is for \( U = 0 \)), one has \( \xi_\lambda = 1 \) whereas when \( |\Psi_\lambda(U)\rangle \) is homogeneously spread over the \( N \) Hilbert space basis states, \( \xi_\lambda \sim N \). To check the above threshold [11], we numerically calculated the PR for the ground-state wavefunction \( |\Psi_0(U)\rangle \). Results obtained from the exact diagonalization of small systems of \( n \leq 8 \) particles are shown in Fig.2. We first note a faster increase of \( \xi_0 \) with \( U \) at larger \( n \) which is not due to an increase of the Hilbert space size as it occurs before a significant portion of the Slater determinant basis starts to be occupied. Most importantly, this increase is exponential (note the vertical log-scale on Fig.2) : fixing e.g. \( U/\Delta = 0.2 \), one gets \( \xi(n) \approx \exp(n/1.6) \). Since each order in perturbation theory gives only an algebraic number of contributions, this exponential increase of the PR cannot be captured by a finite, \( n \)-independent number of orders, and therefore indicates the divergence of the perturbation series as \( n \) increases. Another important feature of Fig.2 is the quite small value \( U \ll \Delta \) at which \( \xi_0 \) starts to increase. This is quite surprising as \( \Delta \) is the only energy scale close to the ground-state. When the PR increases beyond \( \xi_0 \geq 2 \), second (and higher) order terms become more and more important, until eventually perturbation theory breaks down. One can thus extract parametrically the radius of convergence of perturbation theory from the PR by defining a critical interaction strength \( U_c \) from the condition \( \xi_0(U_c) = 2 \). (This choice is arbitrary as long as one chooses a threshold value \( \xi_0(U_c) \) much smaller than the total size of the Hilbert space as this would introduce an artificial \( n \) and \( m \) dependence in \( U_c \).) The inset to Fig.2 shows a \( n- \) (and absence of \( m- \)) dependence of...
$U_c$ clearly confirming (4).

FIG. 2. Ground-state PR $\xi_0$ vs. $U/\Delta$ averaged over 100 (for $n = 8$) to 2000 (for $n = 2$) realizations of Hamiltonian (1) for $m = 16$ and $n=2$. The dotted line indicates the threshold $\xi_0 = 2$. Inset: Critical value of interaction $U_c/\Delta$ necessary to reach $\xi_0 = 2$ vs. $n$, for $m=10$ (triangles), $12$ (+), $14$ (×) and $16$ (circles). The dashed line gives a decay $U_c/\Delta = 0.35/n$.

As yet another check of the threshold (4), we consider the onset of level repulsion for the spacing $s_1 = \xi_1 - \xi_0$ between the ground-state energy $\xi_0$ and the first excited level $\xi_1$. At $U = 0$, this spacing corresponds to a one-body excitation, and considering a randomly distributed one-body spectrum, it is Poisson distributed $P_P(s_1) = \exp(-s_1)$. Switching on $U$ induces off-diagonal matrix elements connecting the two lowest levels and leads to repulsion between them. Making a two-level approximation incorrectly gives the onset of this repulsion at $U = \Delta$. A correct treatment goes as follows. Most terms in the second order contribution (4) are common to both the energies of the ground- and first excited states. The difference corresponds to scattering from or onto the $(n/2)^{\text{th}}$ and $(n/2+1)^{\text{th}}$ orbitals, giving a contribution to the energy difference between the lowest two levels

$$
\sum \frac{(U_{\gamma,\delta})^2}{\epsilon_{\alpha,-n/2} - \epsilon_{\gamma} - \epsilon_{\delta}} - \frac{(U^\gamma,\delta_{+1})^2}{\epsilon_{\alpha,-n/2+1} - \epsilon_{\gamma} - \epsilon_{\delta+1}} \quad (5)
$$

(There is an additional similar contribution arising from the scattering from the $n/2$ and $n/2+1$ orbitals.) We first make the substitution $\sigma((U_{\gamma,\delta})^2 - (U^\gamma,\delta_{+1})^2) = U^2$ for IME fluctuations. Then, and considering an equidistant spacing, a simple counting shows that the number of contributions in the above expression corresponding to a given energy denominator $p\Delta$ grows as $p^2$ up to $p = n/2$ and decreases afterward. Neglecting logarithmic corrections, one gets an estimate for the contributions to the relative fluctuations given by $\sim (U^2/\Delta)n^2$. This estimate can also be obtained by replacing the sums in (6) with integrals. Once these fluctuations become of the order of the spacing between $\xi_0$ and $\xi_1$, $\sim (U^2/\Delta)n^2 \sim \Delta$, an avoided crossing occurs. This signals the onset of level repulsion which therefore occurs at the rate given by (4).

FIG. 3. (a,b,c) Distribution $P(s_1)$ of the first level spacing for 50000 realizations of Hamiltonian (1) with a random distribution of orbitals $e_n$, $m = 14$ (symbols) $n = 3$, $4$, $\ldots$, 7, at an interaction strength $U/\Delta = 1/n$. (a) Shows $P(s_1)$ on a normal scale, (b) its large $s_1$ tail on a semilogarithmic scale and (c) its small $s_1$ behavior on a log-log scale. Empty symbols correspond to odd $n$ and full symbols to even $n$. Clearly, there is an even-odd dependence which is $m$-independent as shown by the superimposed values for $m = 18$ and $n = 3$ (dashed line) and $n = 4$ (dotted-dashed line) on (b) and (c). On (a,b,c) the solid lines show the Poisson and Wigner-Dyson distributions. (d) Shows one realization of the spectrum for Hamiltonian (1) with equidistant one-body spectrum. The spectrum correspond to the full sector $\sigma = 0$ so that level crossings occur between levels with different $\sigma$.

This reasoning is confirmed on Fig.3 (a,b,c) where we present the distribution $P(s_1)$ of the first level spacing for Hamiltonian (1) and different number of particles $n$ at fixed interaction strength $U = \Delta/n$. The two main features that can be seen are : 1) $P(s_1)$ at fixed $U = U_c$ is $n$-independent, except that 2) $P(s_1)$ shows a clear even-odd dependence, in particular there is more level repulsion for odd $n$. This second fact is understood once one realizes that due to SRS, and within a given $(\sigma_\gamma, \sigma)$-block, the first $U = 0$ excitation is doubly degenerate for odd $n$, while it is not degenerate for $n$ even. This results in a stronger effect of the interaction in the former case and the even-odd effect seen on Fig.3 (a,b,c). It is to be stressed that this is purely a spin effect, this even-odd dependence does not appear for spinless fermions. On Fig.3 (d) we also show a plot of the low-lying part of the spectrum which shows an avoided crossing at a value $U/\Delta \approx 0.05$ much too small to be explained by a two-level approximation. We stress that in (d) the
avoided crossing is not accompanied by an increase of the level spacing as would be the case in presence of non-fluctuating IME, and which would delay the breakdown of perturbation theory.

Equation (4) predicts a parametrically small radius of convergence for perturbation theory beyond which the ground-state is composed of exponentially many Slater determinants. It is somehow in opposition with earlier works [1] which, based on extrapolations from higher excitation energies, predicted a border \( \sim \Delta \). The mechanism leading to the breakdown of perturbation theory at higher excitation energies is however due to mixing between two-body levels which are very close in energy, and thus give the dominant contribution in a second order approach. In the immediate vicinity of the ground-state these processes with small denominators do not exist as the lowest energy scale is \( \Delta \) - the approaches used in [12] correspond then to a two-level approximation involving ground- and first excited states. The presented theory show that the correct procedure is to retain a large number of small second order contributions which have an enhanced effect close to the ground-state, as they acquire a well-defined sign and hence add coherently to give the small threshold \( \min \). One has to conclude that the approach used in [12], while fully justified at a sufficient excitation energy, must break down somewhere close to the ground-state.

Random interaction models of the kind investigated here describe interacting systems restricted to energy differences of the order of the Thouless energy \( E_c = g\Delta \). In disordered diffusive systems one has \( E_c = g\Delta \) (\( g \) is the conductance) and introducing a cut-off at \( E_c \) leads to \( m, n \sim g \). From (4) one would expect the breakdown of perturbation theory to occur for \( U_c = \Delta/g \), precisely at the amplitude of fluctuations of IME in these systems [12,13]. The studied model neglects however two ingredients which must be considered when dealing with more realistic systems. First, correlations between IME should play an important role (neglected in the presently studied model) are highly desirable.

Numerical computations were performed at the Swiss Center for Scientific Computing. Work supported by the Swiss National Science Foundation.