

# Nonthermal equilibrium states of closed bipartite systems

Harry Schmidt\* and Günter Mahler

*Institut für Theoretische Physik I, Universität Stuttgart, Stuttgart, Germany*

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We investigate a two-level system in resonant contact with a larger environment. The environment typically is in a canonical state with a given temperature initially. Depending on the precise spectral structure of the environment and the type of coupling between both systems, the smaller part may relax to a canonical state with the same temperature as the environment (i.e., thermal relaxation) or to some other quasiequilibrium state (nonthermal relaxation). The type of (quasi)equilibrium state can be related to the distribution of certain properties of the energy eigenvectors of the total system. We examine these distributions for several abstract and concrete (spin environment) Hamiltonian systems; the significant aspect of these distributions can be related to the relative strength of the local and interaction parts of the Hamiltonian.

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## I. INTRODUCTION

In a composite but closed quantum system in which a smaller central system  $S$  is weakly coupled to a larger environment  $C$ , most of the (pure) states of the total system for a given energy (and possibly some additional constraints) exhibit properties of thermal equilibrium states with respect to the smaller part [1]; i.e., there exists a so-called dominant region in Hilbert space in which the entropy of the central system is close to its maximum value under the given constraints. Therefore, for most pure initial states of the total system, the state of the central system shows decoherence and some kind of thermalization; it typically approaches a quasiequilibrium canonical state with a temperature given by the spectral properties of the environment [2].

If the environment initially is in a thermal state with a given temperature and consists of many bands or of a broad continuum of levels, the central system typically relaxes to a thermal state with the same temperature. This type of relaxation will be called *thermal* relaxation in the following. Here we investigate to what extent certain structures of the total system influence the reached (quasi)equilibrium state. We will relate this equilibrium state to the distribution of the energy eigenvectors of the system, or rather certain important aspects of this distribution. We will show that there is a close relation between the two and how this affects the equilibrium state for different system structures.

We particularly focus on a single spin-1/2 particle coupled to an environment of spin-1/2 particles. Recently, the properties of the spin systems of different structure (rings, stars, and others) have been the subject of extensive interest. A lot of work has been done on the question of entanglement [3–8], their relaxation behavior has been addressed [9,10], and various techniques were suggested to make any spin interact with any other spin [11,12].

Here we extend our analysis from our previous paper [13] regarding the controllability of the relaxation behavior within these spin systems

## II. CANONICAL AND NONCANONICAL RELAXATION

Figure 1 shows a two-level system (TLS) in resonant ( $\delta_S = \delta_C = \delta$ ) contact with an environment consisting of two “energy bands”  $k$  and  $k'$  of degeneracies  $g_k$  and  $g_{k'}$ , respectively (for simplicity we use  $g = g_k$ ,  $g' = g_{k'}$  in the following, typically  $g' > g$ ). The coupling is assumed to be weak; the total system is described by the Hamiltonian

$$\hat{H} = \hat{H}_S + \hat{H}_C + \hat{H}_{\text{int}}.$$

A nonequilibrium state  $|1\rangle_S \otimes |\phi_k\rangle_C$  is depicted (here  $|\phi_k\rangle$  denotes an arbitrary pure environmental state in band  $k$ ).

If this state is taken as the initial state of a Schrödinger time evolution of the total system, a relaxation to an equilibrium situation is expected in which the time-averaged reduced-state operator of  $S$  is given by [1]

$$\hat{\rho}_S = \frac{1}{g + g'} (g'|0\rangle\langle 0| + g|1\rangle\langle 1|), \quad (1)$$

which can be interpreted as a canonical-state operator with inverse temperature:

$$\beta_S = \frac{1}{k_B T} = \frac{1}{\delta_S} \ln \frac{g'}{g}.$$

For a finite environment and weak random coupling, the reduced state of the central system after relaxation still fluctuates around Eq. (1); see [2].

If the central system relaxes to state (1) for any pure state  $|\phi_k\rangle$  of the environment in band  $k$ , it will relax to the same state for an initial state in which the environment is com-

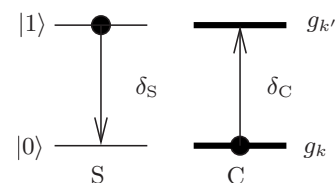


FIG. 1. A two-level system  $S$  in contact with an environment  $C$  consisting of two highly degenerate levels  $k$  and  $k'$  with degeneracies  $g_k$  and  $g_{k'}$ .

\*Electronic address: [harry.schmidt@itp1.uni-stuttgart.de](mailto:harry.schmidt@itp1.uni-stuttgart.de)

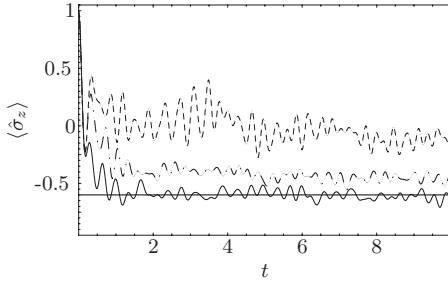


FIG. 2.  $z$  component of the Bloch vector of  $S$  for the initial state depicted in Fig. 1. The environment consists of spins that are randomly coupled to the central spin. Mutual coupling between the environmental spins is strong (bottom curve), weak (middle curve), or nonexistent (top curve). Fluctuations are due to the finite size of the system. The black line indicates canonical equilibrium. The unit of time is of little importance here as it can be adjusted by adjusting the strength of  $\hat{H}_{\text{int}}$ . For additional discussion of the model and the time unit see [13].

pletely mixed within band  $k$ ,  $\hat{\rho}_0 = |1\rangle\langle 1| \otimes \frac{\hat{1}_k}{g}$ . Here  $\hat{1}_k$  denotes the projector onto band  $k$  of the environment.

Assume now that the environment is given by a large number  $N$  of two level systems with a homogeneous Zeeman splitting,  $\hat{H}_C = \sum_{i=1}^N \delta \hat{\sigma}_z^{(i)}$ . The environment initially is taken to be in a thermal state of temperature  $\beta_C$ ,

$$\hat{\rho}_0 = |1\rangle\langle 1| \otimes \frac{1}{Z} e^{-\beta_C \hat{H}_C}.$$

If each band of the environment separately leads to a relaxation into a state (1), the equilibrium state of the central system is given by the canonical state with  $\beta_S = \beta_C$  for large  $N$ . For finite  $N$ , the population of the excited state of  $S$  after relaxation is given by

$$\langle \hat{\rho}_S \rangle_{11} = \frac{N}{N+1} \frac{1}{1 + e^{\delta \beta_C}} + \frac{1}{N+1} \xrightarrow{N \gg 1} \frac{1}{1 + e^{\delta \beta_C}}.$$

Because of this, we call the relaxation from an initial state  $|1\rangle_S \otimes |\phi_k\rangle_C$  to the reduced equilibrium state (1) *canonical* or *thermal* throughout this text.

However, not all environments lead to canonical relaxation of the central system. In [13] we examined several types of spin environments and showed that many of these lead to an equilibrium state that differs from Eq. (1). We call these deviations noncanonical or nonthermal. Figure 2 shows the relaxation behavior for different types of environments. Obviously, not all relax to the same quasiequilibrium state.

### III. ENERGY EIGENVECTOR DISTRIBUTIONS

We now correlate deviations from canonical relaxation with the distribution of the energy eigenvectors of the total system. We only consider the situation depicted in Fig. 1, since environments with more bands in a canonical state can simply be derived from these results. As long as the interaction is weak relative to the band splitting, the total system can be reduced to the subspace consisting of the ‘‘cross states’’

$$\{|0_S, \text{environment in band } k'\rangle,$$

$$|1_S, \text{environment in band } k\rangle\}. \quad (2)$$

In the following we will always refer only to this  $(g+g')$ -dimensional subspace.

Instead of the temperature, we consider the population inversion  $\text{Tr}\{\hat{\sigma}_z \hat{\rho}_S\}$  of the central system for mathematical convenience. The inversion of the canonical state (1) is given by

$$\langle \hat{\sigma}_z \rangle_{\text{can}} = \frac{g - g'}{g + g'}.$$

The energy eigenvectors can be written in the form

$$|\varepsilon\rangle \approx \alpha_\varepsilon |0, \chi_\varepsilon\rangle + \beta_\varepsilon |1, \eta_\varepsilon\rangle, \quad (3)$$

where  $|\chi_\varepsilon\rangle$  is a state in band  $k'$  and  $|\eta_\varepsilon\rangle$  a state in band  $k$  of the environment. In the following we will use  $\varepsilon$  as a discrete index running from 1 to  $g+g'$  to number the energy eigenvectors within the subspace of Hilbert space spanned by the states (2).

We expand the initial state  $\hat{\rho}_0 = |1\rangle\langle 1| \otimes \frac{\hat{1}_k}{g}$  in terms of these eigenvectors,  $\hat{\rho}_0 = \sum_{\varepsilon, \varepsilon'} \rho_{0, \varepsilon \varepsilon'} |\varepsilon\rangle\langle \varepsilon'|$ . Averaging over all times and tracing out the environment yields the equilibrium state of the central system,

$$\bar{\rho}_S = \sum_{\varepsilon} \rho_{0, \varepsilon \varepsilon} \text{Tr}_C\{|\varepsilon\rangle\langle \varepsilon|\} = \sum_{\varepsilon} |\beta_\varepsilon|^2 (|\alpha_\varepsilon|^2 |0\rangle\langle 0| + |\beta_\varepsilon|^2 |1\rangle\langle 1|).$$

The respective inversion is

$$\langle \bar{\sigma}_z \rangle = \sum_{\varepsilon} |\beta_\varepsilon|^2 (|\beta_\varepsilon|^2 - |\alpha_\varepsilon|^2).$$

We notice that

$$\lambda_\varepsilon = |\beta_\varepsilon|^2 - |\alpha_\varepsilon|^2 \quad (4)$$

is the inversion of  $|\varepsilon\rangle$ . Since  $|\beta_\varepsilon|^2 + |\alpha_\varepsilon|^2 = 1$ , we can rewrite the time-averaged inversion of the central system completely in terms of the  $\lambda_\varepsilon$ 's,

$$\langle \bar{\sigma}_z \rangle = \frac{1}{2} \left( \sum_{\varepsilon} \lambda_\varepsilon + \sum_{\varepsilon} \lambda_\varepsilon^2 \right).$$

The first sum can be shown to be equal to  $g-g'$ ; see Appendix A. If we rewrite the second sum in terms of the variance  $\Delta \lambda_\varepsilon^2$  of the  $\lambda_\varepsilon$  distribution, we finally get

$$\langle \bar{\sigma}_z \rangle = \langle \hat{\sigma}_z \rangle_{\text{can}} + \frac{(g+g')}{2g} \Delta \lambda_\varepsilon^2. \quad (5)$$

The average deviation from the canonical equilibrium state is thus mainly given by the distribution of the reduced states of the energy eigenvectors, in particular by its variance.

As long as the width of the distribution is finite, there is always a deviation from the canonical inversion and therefore also from the canonical temperature. For a finite environment this is always the case. We will now consider several types of environments and interactions.





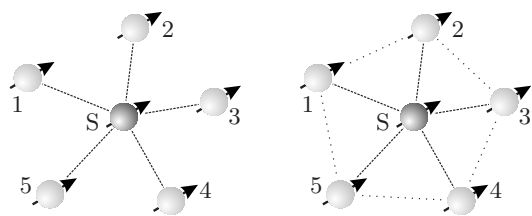


FIG. 9. Schematics of the spin-star (left) and spin-ring (right) configurations. Typically, the environment consists of a lot more than five spins.

equal to the central spin (or almost equal). Due to energy conservation, the system can be reduced to the situation shown in Fig. 1 for each pair of environmental bands. If the environment initially is in a canonical state, we can simply sum up over all bands, as long as the interaction between the environmental spins is small.

The  $\lambda_e$  distributions of several spin environments have been discussed in [13], so we will only discuss them briefly here.

### 1. Spin-star configuration

Figure 9 (left) shows schematically a spin-star configuration—i.e., a central spin coupled to an array of environmental spins without mutual interaction. A typical environment should of course consist of a lot more than five spins. The most general Hamiltonian describing the system-environment interaction is

$$\hat{H}_{\text{int}} = \sum_{i,j=1}^3 \sum_{\nu=1}^N \gamma_{ij}^{(\nu)} \hat{\sigma}_i^{(S)} \otimes \hat{\sigma}_j^{(\nu)}$$

for  $N$  environmental spins.

It has been shown in [13] that if the coefficients  $\gamma_{ij}^{(\nu)}$  are chosen randomly, the initial state depicted in Fig. 4 typically does not relax to the canonical equilibrium state. The Hamiltonian matrix in this case has the form (7); however, with small fluctuations on the diagonal and the interaction part of the Hamiltonian matrix is only sparsely populated. Nevertheless, the  $\lambda_e$  distribution shows some similarity to the one described in Sec. IV B 2 for small level splitting. Figure 10 shows the  $\lambda_e$  distribution for this system.

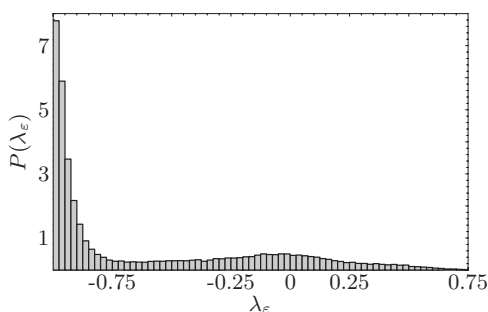


FIG. 10.  $\lambda_e$  distribution for the spin-star configuration. Fourteen environmental spins and the second and third excited bands are considered, corresponding to  $g=91$  and  $g'=364$ .  $\Delta\lambda_e^2 \approx 0.216$ .

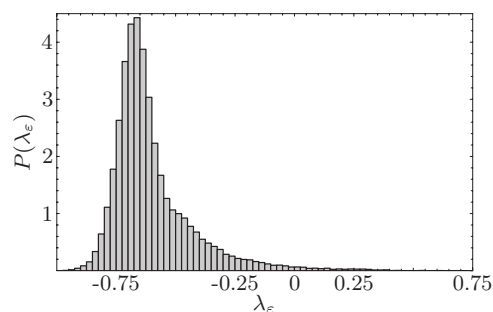


FIG. 11.  $\lambda_e$  distribution for a spin-ring configuration. Fourteen environmental spins and the second and third excited bands are considered, corresponding to  $g=91$  and  $g'=364$ .  $\Delta\lambda_e^2 \approx 0.0295$ .

### 2. Intraenvironmental coupling

If the mutual coupling between the environmental spins is introduced, the situation changes. Figure 9 (right) schematically shows next-neighbor coupling in the environment (spin-ring configuration), but other configurations are possible as well. As long as this coupling is weak, the system can still be considered bandwise.

The interaction typically leads to a level splitting within the bands which in turn leads to a  $\lambda_e$  distribution similar to the one described in Sec. IV B 2 with larger level splitting. Figure 11 shows the  $\lambda_e$  distribution for a spin-ring configuration. The distribution shown is for a  $\hat{\sigma}_x \otimes \hat{\sigma}_x$  next-neighbor coupling. The distributions for different kinds of coupling—e.g., Heisenberg coupling—are similar.

### 3. Inhomogeneous Zeeman splitting

If the individual environmental spins each have a different Zeeman splitting, the situation becomes similar to the one discussed in Sec. IV B 2. Figure 12 shows the  $\lambda_e$  distribution when the Zeeman splittings of the environmental spins are homogeneously distributed within a certain range. The distribution again shows a peak around the mean value  $\bar{\lambda}_e = \langle \hat{\sigma}_z \rangle_{\text{can}}$ , although broader than in the previous case.

## V. WIDTH OF THE DISTRIBUTION AND SPECTRAL WIDTH

Figures 4, 7, and 8 indicate that there is a continuous transition from a situation far from canonical to an almost

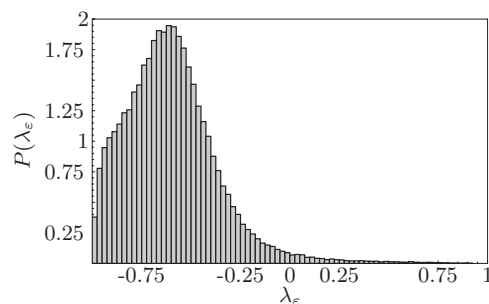


FIG. 12.  $\lambda_e$  distribution for a spin-star configuration with inhomogeneous Zeeman splitting of the environmental spins. Fourteen environmental spins and the second and third excited bands are considered, corresponding to  $g=91$  and  $g'=364$ .  $\Delta\lambda_e^2 \approx 0.0548$ .

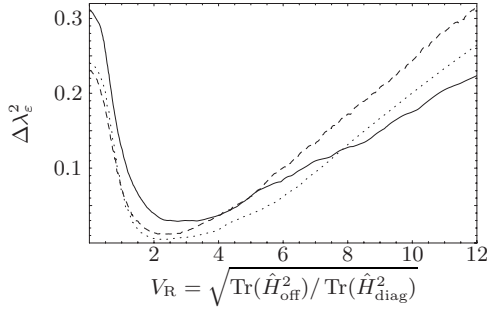


FIG. 13. Variance of the  $\lambda_\varepsilon$  distribution over the relative strength of the environmental spectrum for different types of this spectrum. Solid line: spin-ring with random  $S$ - $C$  coupling. Dashed line: spin-star with random  $S$ - $C$  coupling and inhomogeneous Zeeman splitting within the environment. Dotted line: spin-star with  $XY$  coupling between  $S$  and  $C$  and inhomogeneous Zeeman splitting within the environment.

canonical relaxation, depending on the environmental spectrum. What has been changed is the “strength” of the environmental spectrum from zero to the minimal variance of the  $\lambda_\varepsilon$  distribution. A similar transition can be observed for many different environmental spectra.

In order to relate different types of spectra we split the Hamiltonian matrix (in the considered subspace) in its respective diagonal and off diagonal parts. The off-diagonal part  $\hat{H}_{\text{off}}$  [ $V$  and  $V^\dagger$  of (7)] describes the interaction between central system and environment, while the diagonal part  $\hat{H}_{\text{diag}}$  describes the environmental spectra alone, if system and environment are in resonance. The diagonal part is always taken to be traceless. The quantity we use to compare different spectra is the relative strength of the environmental part to the interaction part,

$$V_R = \sqrt{\frac{\text{Tr}(\hat{H}_{\text{diag}}^2)}{\text{Tr}(\hat{H}_{\text{off}}^2)}}.$$

For a completely random matrix (GUE) this relation is given on average by

$$V_{R,\text{GUE}} = \sqrt{\frac{g^2 + g'^2}{2gg'}},$$

which only depends on  $g/g'$ , not on the actual size of the system.

Figure 13 shows the variance of the  $\lambda_\varepsilon$  distribution for three different types of environmental spectra. In all three cases the environment consists of 14 spins and the second and third excited bands are considered,  $g=91$  and  $g'=364$ , as described in Sec. IV C.

The solid line corresponds to the spin-ring configuration as described in Sec. IV C 2. The intraenvironmental interaction is taken as a  $\hat{\sigma}_x \otimes \hat{\sigma}_x + \hat{\sigma}_y \otimes \hat{\sigma}_y$  next-neighbor coupling; the central system is randomly coupled to each environmental spin. The dashed line corresponds to the configuration described in Sec. IV C 3; there is no mutual interaction between the spins in the environment, but their Zeeman splitting is inhomogeneous. The central system is again coupled

randomly to each environmental spin. The environmental spectrum for the dotted line is the same as for the dashed line. However, the interaction between the central spin and each environmental spin is modeled by  $\hat{\sigma}_x \otimes \hat{\sigma}_x + \hat{\sigma}_y \otimes \hat{\sigma}_y$ . The corresponding average values for a random matrix from the GUE are  $\Delta\lambda_\varepsilon^2 = 2/1425 \approx 0.0014$  and  $V_{R,\text{GUE}} \approx 1.46$ , respectively.

We notice that for each type of coupling and environmental spectrum there is a distinct minimum of  $\Delta\lambda_\varepsilon^2$  for similar values of  $V_R$  close to, but not exactly at, the average value for the GUE matrices.

## VI. CONCLUSION

We have characterized situations under which nonthermal states should result as quasiequilibrium states. For a spin-1/2 particle weakly coupled to a larger environment, there is a close relation between the quasiequilibrium state of the small quantum system coupled to a larger environment and the distribution of certain properties of the energy eigenvectors of the total system. The equilibrium state is directly given by the width of this distribution. The spectral structure of the environment and the exact form of the coupling have a strong influence on the eigenvector distribution. To show this we have considered both abstract system Hamiltonians and Hamiltonians for structured spin environments.

Furthermore, there is a close relation between the width of the  $\lambda_\varepsilon$  distribution and the strengths of both the local (diagonal) and the interaction (off diagonal) part of the Hamiltonian. By changing certain parameters within each system, there is a distinct minimum of the  $\lambda_\varepsilon$  width for a value of the relative strength that is close to the respective value for GUE matrices. This relative strength can thus give an indication whether for a given system relaxation to or close to a thermal state can be expected without calculating the full  $\lambda_\varepsilon$  distribution. The relative width gives an indication how to choose the system parameters properly to achieve a certain type of equilibrium situation. This should be of help when designing a spin system for special (“nonthermal”) relaxation behavior.

### APPENDIX A: TOWARDS Eq. (5)

Here we show that  $\sum_\varepsilon \lambda_\varepsilon = g - g'$ :

$$\begin{aligned} \sum_\varepsilon \lambda_\varepsilon &= \sum_\varepsilon \text{Tr}_S \{ \hat{\sigma}_z^S \text{Tr}_C \langle \varepsilon | \rangle \} = \sum_\varepsilon \text{Tr} \{ (\hat{\sigma}_z^S \otimes \hat{1}^C) | \varepsilon \rangle \langle \varepsilon | \} \\ &= \text{Tr} \{ (\hat{\sigma}_z^S \otimes \hat{1}^C) \}, \end{aligned}$$

the last equality following from the fact that the energy eigenvectors are a complete orthonormal basis in Hilbert space. If we now use the basis  $\{|0, m'\rangle, |1, m\rangle\}$  to calculate the trace ( $m$  and  $m'$  denote the levels in band  $k$  and  $k'$ , respectively), we see that the  $g$  kets  $|1, m\rangle$  yield 1’s, while the  $g'$  kets  $|0, m'\rangle$  yield  $-1$ ’s and the total trace equals  $g - g'$ .

### APPENDIX B: DERIVATION OF Eq. (6)

If we introduce the basis  $\{|k: m\rangle\}$  ( $1 < m \leq g_k$ ) for the band  $k$  and the basis  $\{|k': m\rangle\}$  for the band  $k'$ , we can write the state of the total system as  $(g = g_k, g' = g_{k'})$

$$|\psi\rangle = \sum_{m=1}^{g'} \psi_{0m}|0\rangle \otimes |k':m\rangle + \sum_{m=1}^g \psi_{1m}|1\rangle \otimes |k:m\rangle.$$

The reduced state of the central system becomes

$$\hat{\rho}_S = \text{Tr}_C \hat{\rho} = \sum_{m=1}^{g'} |\psi_{0m}|^2 |0\rangle\langle 0| + \sum_{m=1}^g |\psi_{1m}|^2 |1\rangle\langle 1|.$$

We are interested in the distribution of the inversion of the energy eigenstates of certain Hamiltonians. Since the inversion is determined by the population of each level, we will derive the distribution for the population of the ground state,  $p_0 = \sum_m |\psi_{0m}|^2$ .

For simplicity we introduce a single index  $n$  to label the amplitudes instead of the double index  $0m$  or  $1m$ .  $n$  runs from 1 to  $d = g + g'$  (the reduced Hilbert-space dimension). In this notation,  $p_0 = \sum_{n=1}^{g'} |\psi_n|^2$ .

We now split the amplitudes into real and imaginary parts,  $\psi_n = x_k + ix_{k+1}$ , where  $1 \leq k \leq 2g'$  corresponds to  $|0\rangle \langle 0|$  and  $2g' + 1 \leq k \leq 2d$  corresponds to  $|1\rangle \langle 1|$ ; therefore,  $p_0 = \sum_{k=1}^{2g'} x_k^2$ . The combined probability density of the first  $2g'$  amplitudes

$x_k$  for eigenvectors of random matrices from the GUE is given by [14]

$$P_a(x_1, \dots, x_{2g'}) = \pi^{-1/2} \frac{\Gamma(d)}{\Gamma(d-g')} \left(1 - \sum_{k=1}^{2g'} x_k^2\right)^{d-g'-1}.$$

The desired probability density for the population of the ground state  $p_0$  is given by

$$P_p(p_0) = \int d^{2g'} x P_a(x_1, \dots, x_{2g'}) \delta\left(p_0 - \sum_{k=1}^{2g'} x_k^2\right),$$

integrating over the unit sphere in  $2g'$ -dimensional space. The integral yields

$$P_p(p_0) = \frac{\Gamma(d)}{\Gamma(d-g')\Gamma(g')} p_0^{g'-1} (1-p_0)^{d-g'-1}.$$

Transforming to  $\lambda = 1 - 2p_0$  finally gives the probability density (6),

$$P(\lambda) = \frac{1}{2^{d-1}} \frac{\Gamma(d)}{\Gamma(d-g')\Gamma(g')} (1-\lambda)^{g'-1} (1+\lambda)^{d-g'-1}. \tag{6'}$$

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