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Adiabatic passage through a Feshbach resonance in a degenerate quantum gas

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The dynamics of an adiabatic sweep through a Feshbach resonance in a degenerate quantum gas of fermionic atoms to produce a degenerate quantum gas of diatomic molecules are studied using many-body and mean-field methods. We demonstrate that the dependence of the remaining fraction of atoms Γ on sweep rate α varies from exponential Landau–Zener behaviour for a single pair of particles, to a power-law dependence for a large number of atoms, N. Two different power-law behaviours are obtained depending on the initial molecular fraction. The two different regimes are described in terms of quantum fluctuations: a linear power-law, $\Gamma \propto \alpha$, is obtained when the initial molecular fraction is smaller than the $1/N$ quantum fluctuations, and $\Gamma \propto \alpha^{1/3}$ when it is larger.

1. Introduction

Feshbach resonances have been the driving force behind many of the most exciting experimental achievements in ultra-cold atomic physics in recent years. They are not only a tool for altering the strength and sign of the interaction energy of atoms, they also provide a convenient method for converting atom pairs into molecules, and vice versa. A magnetic Feshbach resonance is a collisional resonance involving pairs of free atoms in the presence of a magnetic field and a bound diatomic molecule state on a different (closed) potential energy surface than the incident (entrance) potential energy surface. The difference in the magnetic moments of the atoms correlating asymptotically at large internuclear distance to the two potential energy surfaces allows the Feshbach resonance to be tuned by changing the magnetic field strength.

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Sweeping the magnetic field as a function of time, so the bound state on the closed channel passes through threshold for the incident open channel from above, can produce bound molecules. This technique for producing molecules from atomic pairs has proved to be extremely effective in converting degenerate fermionic atomic gases containing two different internal spin states to bosonic dimer molecules [1–4]. The reason why fermionic atoms are better candidates than bosonic atoms for such Feshbach sweep experiments is the relatively long lifetimes of the resulting bosonic molecules. The long lifetime of the molecules is due to the Pauli blocking effect which greatly reduces collisions between the molecules consisting of fermionic atoms and other fermionic atoms in the gas [5].

This paper focuses on the molecular production efficiency of such adiabatic Feshbach sweep experiments. We determine the functional dependence of the remaining atomic fraction Γ on the Feshbach sweep rate α. We follow the ideas presented in our paper [6], extending the calculations, and presenting a more detailed account of the theoretical considerations for treating the dynamics of ultra-cold Feshbach sweep experiments.

In the fermionic Feshbach sweep experiments [1–4], the Fermi energy is the smallest energy scale in the system. Hence, we treat the fermions theoretically as occupying the lowest possible many-body state consistent with symmetry considerations arising from their method of preparation, i.e. we assume that the quantum states are filled up to the Fermi energy in a fashion consistent with the symmetry properties of the gas. In this sense, the gas can be thought of as a zero temperature gas.

For a single pair of fermionic atoms in a Feshbach sweep experiment, the Landau–Zener (LZ) model [7] is the paradigm for explaining how transitions occur. Theoretical interpretation of experimental results for the molecular production efficiency in Feshbach sweep experiments in a gas have been based on Landau–Zener theory [8]. Experimental molecular efficiency data has been fit by an exponential form. Figure 1 shows the experimental data (black squares) of [2] fit by an exponential function (dashed curve), $\Gamma = 0.479 \exp(-\alpha/1.3) + 0.521$, as suggested in [2]. However, the data can be fit to the same level of accuracy by a power-law dependence (green curve). Note that the original experimental data saturated at a remnant of 1/2 contrary to the expected LZ behaviour. This discrepancy has been previously explained [9] employing symmetry arguments appropriate for the method of preparation of the initial state of the gas before the Feshbach sweep. Here we describe how the LZ theory fails for a degenerate quantum gas of fermionic atoms when the number of atoms is large and the power-law dependence of figure 1 emerges. We also predict two different power-law behaviours, $\Gamma \propto \alpha$ and $\Gamma \propto \alpha^{1/3}$, depending on the initial state of the system prior to the Feshbach sweep.

The paper is organized as follows. In section 2 we introduce the model, the atom–molecule Feshbach Hamiltonian and the main approximations used. In section 3 we discuss the mean-field approximation, the power-law dependences obtained and the role of quantum fluctuations which lead to the linear dependence of the molecular production efficiency on the sweep rate. Finally, in section 5 we summarize our work, comparing it with other theoretical studies which have obtained similar power-law dependences.

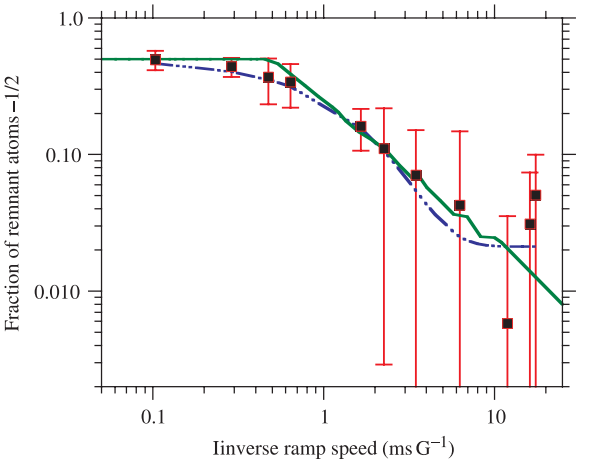

Figure 1. Fraction of remnant atoms, Γ, vs. inverse ramp speed $1/\dot{B}$ across the 543 G resonance of ^{6}Li. The experimental data (black squares) of [2], which saturates at a remnant fraction of 1/2 [9], and the mean-field calculations obey a linear dependence on sweep rate beyond 0.5 ms G^{-1}. $g^2/\alpha N$ is multiplied by 0.5 ms G^{-1} to scale the abscissa for the calculated results. Also shown as a dashed line is the best exponential fit to the data, $\Gamma = 0.479\exp(-\alpha/1.3) + 0.521$ as suggested in [2]. (The colour version of this figure is included in the online version of the journal.)

2. The model

Whereas the experimental findings for molecular production in broad Feshbach resonances that are swept with a very slow sweep rate [3, 4] are well explained employing a thermodynamic model wherein thermodynamic equilibrium is assumed, the narrow ^{6}Li resonance that is traversed with sweep rates that are much more rapid is not expected to fit such a description. For the experiment performed by Strecker *et al.* on the narrow ^{6}Li Feshbach resonance [2], we expect that there is a wide range where atoms and molecules coexist, forming a coherent state. We consider the temperature equal to the zero limit to explain the experimental data. The sweep rate in the above experiment is considered to be adiabatic with respect to both the many-body state as well as the single-particle timescales, allowing us to consider the collisionless regime in which inelastic collisions can be ignored. At low temperatures we assume a single bosonic mode Hamiltonian [10–16] because of the Cooper instability which singles out the zero momentum mode of the molecules produced. Thus, we take the Hamiltonian to be

$$H = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \mathcal{E}(t) b_0^{\dagger} b_0 + g\left(\sum_{\mathbf{k}} c_{\mathbf{k},\uparrow} c_{-\mathbf{k},\downarrow} b_0{}^{\dagger} + H.c.\right), \tag{1}$$

where $\epsilon_{\mathbf{k}} = \hbar^2 k^2/2m$ is the kinetic energy of an atom with mass m and g is the atom–molecule coupling strength. The molecular energy $\mathcal{E}(t) = \alpha t$ is linearly swept at a rate α through resonance to induce adiabatic conversion of fermi atoms to

bose molecules. The annihilation operators for the atoms, $c_{\mathbf{k},\sigma}$, obey fermionic anti-commutation relations, whereas the molecule annihilation operator b_0 obeys a bosonic commutation relation.

One can also further simplify the Hamiltonian by neglecting the fermionic dispersion. This approximation has been commonly used [8, 11] and accounts for the use of a simple two-level LZ model, as opposed to a multilevel one, for such systems. To justify this assumption we have conducted exact numerical simulations to determine the effect of fermionic dispersion on the adiabatic conversion efficiency. Figure 2 shows exact numerical results for the adiabatic conversion of five atom pairs into molecules, for different values of the atomic level spacing (and hence of the Fermi energy E_{F}). It demonstrates that the *final* adiabatic conversion efficiency is completely insensitive to the details of the atomic dispersion. It is evident that, while the exact dynamics depends on E_{F}, and the levels are sequentially crossed as a function of time as the bound state crosses the level energies, the same final efficiency is reached regardless of the atomic motional timescale (i.e. regardless of level spacing). In particular, the figure shows that in the limit as $\alpha \to 0$ it is possible to convert *all* atom pairs into molecules. This is a unique feature of the nonlinear parametric coupling between atoms and molecules, which should be contrasted with a marginal conversion efficiency expected for linear coupling in the multi-level LZ model.

Employing the degenerate model with $\epsilon_{\mathbf{k}} = \epsilon$ for all $\mathbf{k}$ [14–16], it is convenient to define the model in terms of the following lowering and raising operators [15, 17]:

$$\mathcal{J}_- = \frac{{b_0}^\dagger \sum_{\mathbf{k}} c_{\mathbf{k},\uparrow} c_{-\mathbf{k},\downarrow}}{(N/2)^{3/2}}, \quad \mathcal{J}_+ = \frac{\sum_{\mathbf{k}} c^\dagger_{-\mathbf{k},\downarrow} c^\dagger_{\mathbf{k},\uparrow} b_0}{(N/2)^{3/2}}, \quad \mathcal{J}_z = \frac{\sum_{\mathbf{k},\sigma} c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} - 2{b_0}^\dagger b_0}{N}, \tag{2}$$

where $N = 2{b_0}^\dagger b_0 + \sum_{\mathbf{k},\sigma} c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}$ is the conserved total number of particles. It is important to note that $\mathcal{J}_-, \mathcal{J}_+, \mathcal{J}_z$ do not span $SU(2)$, since the commutator

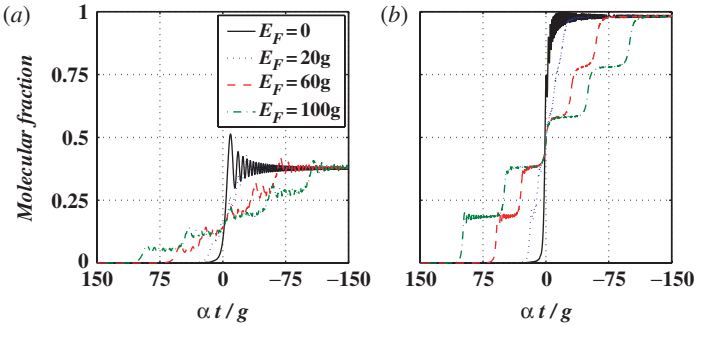

Figure 2. Many-body collective dynamics of adiabatic passage from a fermionic atomic gas into a molecular Bose–Einstein condensate (BEC) for five pairs of fermionic atoms. (*a*) Sweep rate $\alpha = 2g^2N$. (*b*) Sweep rate $\alpha = g^2N/4$. Overall efficiency is independent of atomic dispersion in both (*a*) and (*b*). (The colour version of this figure is included in the online version of the journal.)

$[\mathcal{J}_+, \mathcal{J}_-]$ yields a quadratic polynomial in $\mathcal{J}_z$, despite the fact that the commutators $[\mathcal{J}_+, \mathcal{J}_z]$ and $[\mathcal{J}_-, \mathcal{J}_z]$ have the right commutation relations. The operators $\mathcal{J}_x = \mathcal{J}_+ + \mathcal{J}_-$ and $\mathcal{J}_y = -\mathrm{i}(\mathcal{J}_+ - \mathcal{J}_-)$ can also be defined. Up to a c-number term, Hamiltonian (1) takes the form

$$H = \frac{N}{2}\left(\Delta(t)\mathcal{J}_z + g\frac{N^{1/2}}{2}\mathcal{J}_x\right), \tag{3}$$

where $\Delta(t) = 2\epsilon - \mathcal{E}(t)$. Defining a rescaled time $\tau = N^{1/2}gt$ and assuming a filled fermi sea, we obtain the Heisenberg equations of motion for the association of a quantum-degenerate gas of fermions,

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}\tau}\mathcal{J}_x &= \delta(\tau)\mathcal{J}_y, \\
\frac{\mathrm{d}}{\mathrm{d}\tau}\mathcal{J}_y &= -\delta(\tau)\mathcal{J}_x + \frac{3(2^{1/2})}{4}(\mathcal{J}_z - 1)\left(\mathcal{J}_z + \frac{1}{3}\right) - \frac{2^{1/2}}{N}(1 + \mathcal{J}_z), \\
\frac{\mathrm{d}}{\mathrm{d}\tau}\mathcal{J}_z &= 2^{1/2}\mathcal{J}_y,
\end{aligned} \tag{4}$$

which depend on the single parameter $\delta(\tau) = \Delta(t)/N^{1/2}g = (\alpha/g^2N)\tau$. It is interesting to note that exactly these equations of motion are obtained for the two-mode atom–molecule BEC [17] where, for the bosonic case, raising and lowering operators are defined as

$$\mathcal{J}_- = \frac{{b_0}^\dagger a_1 a_2}{(N/2)^{3/2}}, \quad \mathcal{J}_+ = \frac{a_2^\dagger a_1^\dagger b_0}{(N/2)^{3/2}}, \quad \mathcal{J}_z = \frac{2{b_0}^\dagger b_0 - \sum_{\mathbf{k},\sigma} a_{\mathbf{k},\sigma}^\dagger a_{\mathbf{k},\sigma}}{N}, \tag{5}$$

where a_1 and a_2 are bosonic annihilation operators obeying bosonic commutation relations. In these definitions, the sign of the operator $\mathcal{J}_z$ has been reversed relative to equation (2), and therefore this maps fermionic association to bosonic dissociation. This provides another perspective on the recently observed mapping between the two systems [14–16].

3. Mean-field approximation and the effects of fluctuations

The mean-field limit of equations (4) is given by replacing $\mathcal{J}_x$, $\mathcal{J}_y$ and $\mathcal{J}_z$ by their expectation values u, v and w which correspond to the real and imaginary parts of the atom–molecule coherence and the atom–molecule population imbalance, respectively. Since quantum fluctuations in $\mathcal{J}_z$ are of order $1/N$, it is also consistent to omit the quantum noise term $2^{1/2}(1 + \mathcal{J}_z)/N$ as long as $\mathcal{J}_z$ is of order 1. For small w however, when the molecular population is of the order of its quantum fluctuations, this quantum term becomes dominant and will have a significant effect on sweep efficiency, as will be shown below.

In the classical field limit, the equations of motion

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\tau}u &= \delta(\tau)v,\\ \frac{\mathrm{d}}{\mathrm{d}\tau}v &= -\delta(\tau)u + \frac{3(2^{1/2})}{4}(w-1)\left(w+\frac{1}{3}\right),\\ \frac{\mathrm{d}}{\mathrm{d}\tau}w &= 2^{1/2}v,\end{aligned} \tag{6}$$

depict the motion of a generalized Bloch vector on a two-dimensional surface corresponding to the conservation of single-pair atom–molecule coherence, in analogy to the motion of the Bloch vector on the Bloch sphere for the paradigm two-level system.

So far, we have neglected the effect of quantum fluctuations, which may be partially accounted for by the c-number limit of the source term $(2^{1/2}/N)(1+\mathcal{J}_z)$ in equations (4). As a result, we found that $\dot{w}_0$ does not vanish as w_0 approaches 1. Consequently, the remaining atomic population is expected to scale as the cubic root of the sweep rate if the initial average molecular fraction is larger than the quantum noise. However, starting purely with fermion atoms (or with molecules made of bosonic atoms), corresponding to an unstable fixed point of the classical phase space, fluctuations will serve to trigger the association process and will thus initially dominate the conversion dynamics.

In order to verify that such quantum fluctuations can be accurately reproduced by a 'classical' noise term near $w=1$, we compare the onset of instability from exact many-body calculations to the onset of mean-field instability according to the revised mean-field equations.

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\tau}u &= \delta(\tau)v,\\ \frac{\mathrm{d}}{\mathrm{d}\tau}v &= -\delta(\tau)u + \frac{3(2^{1/2})}{4}(w-1)\left(w+\frac{1}{3}\right) + \frac{2^{1/2}}{N}(1+w),\\ \frac{\mathrm{d}}{\mathrm{d}\tau}w &= 2^{1/2}v,\end{aligned} \tag{7}$$

where we have retained the $\mathcal{O}(1/N)$ noise term $(2^{1/2}/N)(1+w)$. We have checked to make sure that there is excellent agreement in the early-time dynamics, indicating that the mean-field noise term gives the correct behaviour near the instability point.

We have analysed the dynamics of the mean-field treatment using action-angle variables and direct numerical simulation [6]. This analysis shows that equations (6) yields the following dependence of the remnant fraction of atoms as a function of sweep rate,

$$\Gamma \equiv 1 - w(t\to\infty) \propto \alpha^{1/3}, \tag{8}$$

whereas equations (7) yields

$$\Gamma \propto \alpha. \tag{9}$$

Equations (8) and (9) constitute the main results of this work. We predict that the remnant atomic fraction in adiabatic Feshbach sweep experiments will scale as a power law with sweep rate due to the curve crossing in the nonlinear case. When the system is allowed to go near the critical point (i.e. when $1 - w_0(t_i) \ll 1/N$) quantum fluctuations are the major source of non-adiabatic corrections, leading to a linear dependence of the remnant atomic fraction on the sweep rate. We note that a similar linear dependence was predicted for adiabatic passage from bosonic atoms into a molecular BEC [18]. When the the initial state is such that it has already a large molecular population (i.e. for $1 - w_0(t_i) \gg 1/N$) and fluctuations can be neglected, we obtain a cubic-root dependence of the the final atomic fraction on sweep rate.

4. Numerical many-body results

To confirm the predictions of section 3, we carried out exact many-body numerical calculation for particle numbers in the range $2 \leq N \leq 800$, by Fock-space representation of the operators $\mathcal{J}_i$ and direct propagation of the many-body equations (4), according to the methodology of [14]. Figure 3 shows Γ versus dimensionless inverse sweep rate $g^2/\alpha N$. The exact calculations are compared with a mean-field curve (solid green line), computed numerically from the mean-field equations (6). The log–log plot highlights the mean-field power-law dependence, obtained in the slow ramp regime $\alpha < g^2 N$, whereas the log–linear insert plot demonstrates exponential behaviour. For a single pair of particles, $N = 2$, the quantum association problem is

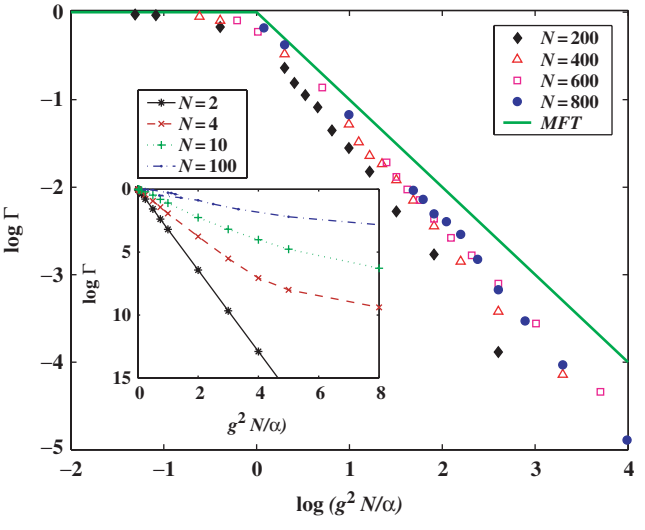

Figure 3. Many-body calculations for the fraction of remnant atoms, Γ, Vs. dimensionless inverse sweep rate for various particle numbers in the range $N = 2$ to 800. The many-body results for a large number of particles converge to the mean-field results (solid green line) computed numerically from the mean-field limit of equations (4). (The colour version of this figure is included in the online version of the journal.)

formally identical to the linear LZ paradigm, leading to an exponential dependence of Γ on sweep rate (see insert of figure 1). However, as the number of particles increases, many-body effects come into play, and there is a smooth transition to a power-law behaviour in the slow ramp regime $\alpha < g^2N$. The many-body calculations converge to the mean-field limit, corresponding to a linear dependence of Γ on α, as predicted in equation (9).

The results of figure 3 prove the convergence of many-body calculations to the mean-field theory used as a basis to our analysis in previous sections. Having established the validity of this classical field theory, and numerically confirmed the appearance of power-law behaviour, we return to the experimental results of [2] shown in figure 1. Comparison of our mean-field numerical calculation with the experimental data (red squares in figure 1) clearly shows good agreement. However, since an equally good exponential fit can be found [2], as shown in figure 1, current experimental data does not serve to determine which of the alternative theories is more appropriate. We have obtained similar agreement with the experimental data of [1], but data scatter and error bars are again too large to conclusively resolve power laws from exponentials. Further precise experimental data for slow ramp speeds and different particle numbers will be required to verify or to refute our theory.

5. Summary and discussion

In summary, we have shown that nonlinear many-body effects can play a significant role in the atom–molecule conversion process for degenerate fermionic atomic gases. The many-body nature of the dynamics (and its resulting nonlinear dynamics manifestation in mean-field dynamics) modifies the LZ exponential dependence on sweep rate, turning the functional behaviour on sweep rate into a power law. Though the experimental data was originally fit with LZ exponential behaviour [2], we have demonstrated that it can be fit just as well with a power-law dependence. Hopefully, future experimental work will be able to determine which fit is best at low temperatures; a larger range of sweep rates will be necessary for this purpose.

The realization that many-body effects can modify LZ behaviour, producing power law behaviour has been predicted by several other groups in different contexts. For the theory of Josephson tunneling [19, 20] as well as for a BEC in a double potential well or in an optical lattice, power-law behaviour (a 3/4 power) was predicted by Liu *et al*. [19]. In this paper, as well as in our previous work [6] we employed the theoretical techniques developed by Liu *et al*., modifying them for the case of a non-spherical two-dimensional phase space surface. The bosonic photo-association problem was addressed by Ishkhanyan *et al*. [18]; this is simply the bosonic analogue of the fermionic pairing we addressed in this paper. Given the mapping between the bosonic disassociation to fermionic association [14–16], it is not surprising that Ishkhanyan *et al*. obtained a linear power law result. However the semiclassical approximation method they used to solve the problem required them to assume that the system starts as all atoms at large negative detuning. Assuming that the initial condition is all atoms inherently includes the quantum fluctuation resulting

in only the linear dependence. In such a method it is impossible to separate the effects of quantum fluctuations. Altman and Vishwanath [21] studied rapid sweeps across a Feshbach resonance; they called this a dynamic projection on Feshbach molecules. They state that a fast sweep can be approximated by a sudden part followed by an adiabatic time evolution part. In their paper [21] they obtain the same linear and 1/3 power laws and use a spatial argument to explain them. Their argument assumes that at some stage that the sweep becomes fast and then atom pairs are projected onto molecules. The power law results from the spatial overlap of a molecular wave function with that of a pair of atoms. For a Cooper pair, this leads to the 1/3 power law due to the specific spatial form of the Cooper pair, whereas the projection of a random pair of atoms onto a molecule gives a linear dependence. Finally in a recent paper, Barankov and Levitov [22] study the same problem of dynamical atom/molecule projection, for fermion pairing into bosonic molecules using a different method (a variant of the Wiener–Hopf method) and obtained the same power laws. With respect to all these approaches we should stress our new results. We have demonstrated how exponential LZ behaviour, applicable to two atoms, is transformed into a power-law dependence (see figure 3) as the number of atoms increases (for a coherent zero temperature gas). We have shown numerically that the efficiency of molecular production is independent of fermionic dispersion (see figure 2). Our simple mean-field theory allowed us to discriminate between the linear and one third power-law dependencies and enabled us to give a clear explanation of how these results depend on quantum fluctuations. In showing that the fermionic equations of motion (4) are the same for operators built for the bosonic case (5), we have explicitly demonstrated the mapping between fermion association and bosonic dissociation on the operator level. Finally, as mentioned above, we fit experimental low temperature Feshbach sweep data with a power-law dependence (see figure 1).

Acknowledgments

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