Dynamical universality class of Brownian motion and exact results for a single-impurity $s=\frac{1}{2}$ XY chain

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Relaxation phenomena in a class of nondissipative systems with two highly disparate time scales (i.e., Brownian systems) have unique commonalities quantifiable via two scalars. It is shown that the *exactly* solvable problem of the dynamics of a *weakly linked* impurity spin in a $s=\frac{1}{2}$ XY chain belongs to this dynamical universality class and so does that of a heavy mass in an infinite harmonic oscillator chain and a spinless quasi two-dimensional *attractive* Fermi gas in the long-wavelength limit. The case of the strongly linked impurity in the XY chain is also discussed along with the corresponding limits in the harmonic oscillator chain and the electron-gas problems.

According to the continued-fraction formalism[1] (CFF) for relaxation studies[2,3] one can *uniquely specify* the behavior of some dynamical variable in the time domain of any Hermitian (i.e., nondissipative) system using two scalar quantities, d and σ. These quantities specify the dimensionality and the hypersurface, respectively, of a certain Hilbert space in which the dynamical variable of interest, say $A(t)$, resides. As the vector $A(t)$ evolves in time according to the appropriate equation of motion (i.e., Heisenberg equation for quantum systems and Liouville equation for classical systems), its tip traces out the hypersurface σ. Thus, knowledge of d, the dimensionality of the Hilbert space, and σ, the shape of the Hilbert space, is in principle, sufficient to characterize the dynamical correlations (i.e., relaxation functions) involving $A(t)$ for a given system.

As we shall see, seemingly unrelated dynamical variables in very different physical systems may exhibit the same d and σ and hence in that specific sense may belong to the same *dynamical universality class* (DUC).[5] Physical problems in the same DUC exhibit identical relaxation *at all times*. Such knowledge may lead to previously unnoticed deep connections between the physical systems in the same DUC and is hence of significant scientific interest.

It is well known for instance, that both the $s=\frac{1}{2}$ XY and transverse Ising (TI) models in one-dimensional (1D) can be reduced to the free fermion problem.[4] Subsequently, starting from the Hamiltonians for the XY and TI chains, with appropriate choice of parameters and with careful considerations regarding system symmetry, it has been shown that the time evolutions of any bulk spin in these systems, in the thermodynamic limit, are identical, and hence they belong to the same DUC.[6] Spin dynamics, however, is sensitive to the existence of translational invariance. A few years ago, it was proved that the dynamics of the surface spin in a semi-infinite XY chain is closely related (though not exactly equivalent) to that in an infinite harmonic oscillator chain.[7] This work showed that the breaking of translational invariance allows one to readily probe the simplest possible ways for excitation to propagate in an XY chain (this propagation is already quite involved for the Heisenberg chain). Hence, one may expect that spin chains with a single magnetic impurity may exhibit simpler dynamical behavior for the impurity spin and those spins in its vicinity than the dynamical behavior exhibited by the bulk spins.

The physical properties of extremely low impurity quantum spin systems, especially the single impurity $s=1/2$ Heisenberg chain and its relation to the one-impurity Kondo problem, have attracted considerable attention within the past few years.[8] In this paper we demonstrate that the dynamical xx (or yy) correlations of the impurity spin in a $s=\frac{1}{2}$ XY chain with a single weakly bound magnetic impurity is *dynamically equivalent* to two very different problems.[5] These are (i) the velocity relaxation of a heavy mass impurity in an infinite harmonic oscillator chain (i.e., a slightly modified version of the "Brownian motion" problem),[9] and (ii) the density relaxation in a quasi-2D attractive quantum fermion gas at temperature $T=0$.[10] The most important commonality between these systems is that they all have two highly disparate characteristic time scales, just like what one finds in Brownian motion.[11] Hence, we contend that these systems belong to the dynamical universality class of Brownian motion.

The calculation of a dynamical spin pair-correlation function, $\langle S_j^\alpha(t)S_j^\alpha\rangle/\langle(S_j^\alpha)^2\rangle$, where $\alpha=(x,y)$ for a single impurity $s=\frac{1}{2}$ XY chain with j being the impurity spin, has been accomplished as follows.[12] The CFF provides a prescription for constructing solutions to the Heisenberg equation of motion for some dynamical variable and in turn for calculating the dynamical spin pair correlations involving the dynamical variable under study. Using the CFF we first express the operator $S_j^\alpha(t)$ as an orthogonal expansion in a Hilbert space. It is assumed[2] that the Hilbert space is spanned by a complete set of orthogonal bases with the orthogonality being realized via a suitable scalar product, e.g., the Kubo scalar product (KSP).[1] Thus,

$$S_j^\alpha(t)=\sum_{\nu=0}^{d-1} f_\nu a_\nu(t), \tag{1}$$

where f_ν's form a complete set of *time-independent* orthogonal bases and $a_\nu(t)$'s are their *time-dependent coefficients*.

The orthogonality of the f_ν's are realized through the KSP which leads to a simple recurrence relation (RR), RR I, for the f_ν's given by

$$f_{\nu+1}=\frac{i}{\hbar}[H,f_\nu]+\Delta_\nu f_{\nu-1}, \tag{2}$$

where the square braces denote commutators and $\Delta_\nu=(f_\nu,f_\nu)/(f_{\nu-1},f_{\nu-1})$, $\nu\geqslant 1$, and for this problem in which spin dynamics in the temperature $T\to\infty$ limit is considered we choose $(X,Y)\equiv\langle XY^\dagger\rangle-\langle X\rangle\langle Y^\dagger\rangle$ (a special case of the KSP). From here on we set $\hbar\equiv 1$ for convenience. Since Eqs. (1) and (2) must satisfy the Heisenberg equation of motion for $S_j^\alpha(t)$ one obtains a second RR, RR II, concerning the $a_\nu(t)$'s,

$$\Delta_{\nu+1}a_{\nu+1}=-\frac{da_\nu}{dt}+a_{\nu-1},\quad \nu\geqslant 0,\quad a_{-1}\equiv 0. \tag{3}$$

A more convenient way of writing RR II, for practical applications,[13] is by taking its Laplace transform and thereafter expressing $a_0(z)$ as a continued fraction (CF). For ergodic problems, $d\to\infty$ in Eq. (1),[14] and hence $a_0(z)$ is an infinite CF (ICF) as described below

$$a_0(z)=1/(z+\Delta_1/\{z+\Delta_2/[z+\Delta_3/(z+\cdots\ \text{ to }\ \infty)]\}). \tag{4}$$

Since $a_0(t)=4\langle S_j^\alpha(t)S_j^\alpha\rangle$ at $T=\infty$, it follows from Eq. (4) that the information for the calculation of the dynamical spin pair correlation is contained in $\{\Delta_\nu\}$, where the Δ_ν's are functions of multipoint static correlations of the system.[7] The calculation of the Δ_ν's is greatly simplified at high T's at which the traces over the spins that enter into the Δ_ν's become trivial to evaluate. The resultant dynamics which, however, remains highly nontrivial, describes a system in which all the eigenstates are nearly equally Boltzmann weighted (unless $T=\infty$ when all the states are *precisely* equally weighted). In what follows we sketch the exact solution for $a_0(t)=4\langle S_j^x(t)S_j^x\rangle$ for the $s=1/2$ XY chain with a single magnetic impurity at site j in the limit of weak coupling at $T=\infty$. We then show, that $\sigma\equiv\{\Delta_1,\Delta_2,\Delta_3,\ldots\}$ for this spin problem is identical to that for velocity autocorrelation function of a heavy impurity in an infinite harmonic oscillator chain[5,11] and that for density relaxation in a 2D quantum electron gas of attractive (abnormal) fermions in the long-wavelength limit at $T=0$.[5,10]

Single impurity $s=\frac{1}{2}$ XY chain: This system can be described by the following Hamiltonian:

$$H=\sum_{i\neq j,i=1}^{N}\vec{S}_i\cdot\vec{S}_{i+1}+\alpha\vec{S}_j\cdot(\vec{S}_{j-1}+\vec{S}_{j+1}), \tag{5}$$

where $\vec{S}_k\equiv(S_k^x,S_k^y)$ in the XY chain and the impurity spin which is coupled to its nearest neighbors via the dimensionless quantity α, has been labeled as the jth spin and $N\to\infty$. The sign of the coupling constant in Eq. (5), which is set to unity, is unimportant for our analysis which will be carried out at $T=\infty$. To study $S_j^x(t)$, i.e., the dynamics of the impurity spin, for the Hamiltonian in Eq. (5), we choose $f_0=S_j^x(0)\equiv S_j^x$. This choice is consistent with the spirit of linear-response theory in which one probes the spreading of an infinitesimal perturbation throughout the system. Using RR I in Eq. (2), $T=\infty$ and, for the present, retaining only the lowest-order terms in α we find,

$$\frac{f_\nu}{\alpha}=\phi(\nu)(S_{j-\nu}^xS_{j-(\nu-1)}^z\cdots S_j^z+S_{j+\nu}^xS_{j+(\nu-1)}^z\cdots S_j^z),$$

$$\nu(\neq 0)=\text{even}, \tag{6}$$

$$\frac{f_\nu}{\alpha}=\phi(\nu)(S_{j-\nu}^yS_{j-(\nu-1)}^z\cdots S_j^z+S_{j+\nu}^yS_{j+(\nu-1)}^z\cdots S_j^z),$$

$$\nu(\neq 0)=\text{odd}, \tag{7}$$

where $\phi(\nu)=(+,-,-,+,+,-,-,+,+,\ldots)$ for $\nu=1,2,3,\ldots\infty$. At $T=\infty$, recalling the definition of Δ_ν [see below Eq. (2)], this implies that

$$\Delta_1=\frac{\alpha^2}{2},\quad \Delta_\nu=\frac{1}{4},\nu>1, \tag{8}$$

and hence $\sigma=(\alpha^2/2,1/4,1/4,\ldots)$. If all the Δ_n's were the same, σ would have described the surface of a hypersphere. Hence, one can regard the present σ as one which describes the hypersurface of a "distorted" hypersphere. This distortion can be readily attributed to the weakened bonds [characterized by $\alpha\ll 1$ in Eq. (5)] joining the nearest neighbors of the impurity in real space which contributes to the *slow* time scale in this problem. The rest of the scalars enter from the existent *fast* time scale associated with the dynamics of the other spins which are coupled between the nearest neighbors by the coupling constant which is set to unity. The ICF for this problem can be trivially summed and the result is

$$a_0(z)=\frac{1}{z(1-\alpha^2)+\alpha^2\sqrt{z^2+1}}, \tag{9}$$

where only the positive sign between the two terms in the denominator is relevant to insure that z is imaginary. Hence, upon inverse Laplace transform of $a_0(z)$ in Eq. (9), $a_0(t)=1/2\pi i\int_C dz\,\exp(zt)a_0(z)$, where the contour C runs along the right side of the imaginary axis from $-i\infty$ to $i\infty$. This integral cannot be evaluated in closed form.[2,11] For $\alpha\to 0$, $t\to\infty$ $a_0(t)$ has been expressed exactly by several workers.[11] They have shown that $a_0(t)$ consists of an *exponentially decaying* (Brownian motion) part and an *oscillatory algebraically decaying* part. Hence, at large times (e.g., typically $t\sim 10^2$, for $\alpha\sim 1/10$ and large time depends upon how small α is as discussed in Sen *et al.* in Ref. 11), it is the slower algebraic decay that dominates the relaxation process. Rigorously one can show that,[5]

$$a_0(t)=\frac{\alpha^2}{\pi|(2\alpha^2-1)|}\sum_{n=1}^{\infty}\left[\frac{2(1-\alpha^2)}{(1-\alpha^2)^2}\right]^n\Gamma\left(n+\frac{1}{2}\right)\frac{J_n(t)}{t^n}, \tag{10}$$

where $\alpha\to 0$, Γ and J_n are gamma and Bessel functions, respectively, and time t is expressed in units of the coupling constant in Eq. (5) which is set to unity. The behavior looks markedly exponential-like until as $t\to\infty$, it acquires $t^{-3/2}\cos(t-\pi/4)$ (see Fig. 1 in Sen *et al.* in Ref. 11). It may be noted that knowing $\{f_\nu\}$, $a_0(t)$ and $\{\Delta_\nu\}$ one may readily solve[7] for all the quantities in Eq. (1) and hence solve for the Heisenberg equation of motion $S_j^x(t)$.[15]

Harmonic oscillator chain with a heavy impurity: As mentioned earlier, σ for an infinite harmonic oscillator chain characterized by

$$H=\sum_{i=-N}^{N}\frac{p_i^2}{2m_i}+\frac{k}{2}\sum_{i=-N}^{N}(x_{i+1}-x_i)^2, \tag{11}$$

where p_i, x_i denote the momentum, position of oscillator i, $m_i=m$ if $i\neq 0$ and $m_i=m_0$ if $i=0$ with $m_0\gg m$ is a solved problem.[11] The Hilbert space of the velocity $v_0(t)$ of the heavy impurity at site 0 admits the following $\sigma=(2\lambda,1,1,\ldots)$, where $\lambda=m/m_0$. For $m/m_0=\lambda\to 0$, the hypersurface of the Hilbert space for the velocity of the impurity mass is *identical* (to within a constant) to that of the impurity spin in the $s=\frac{1}{2}$ XY chain for $\alpha\to 0$. This equivalence may be viewed as follows.

The key issue is that the characteristic frequency $\omega_0\equiv 2\sqrt{k/m_0}$ associated with the motion of the heavy mass, m_0, in the harmonic oscillator chain is vanishingly small compared to the frequencies characterizing the dynamics of all the other masses for $\lambda\to 0$ and hence ω_0 fixes the macroscopic time scale. Thus, there are two highly disparate time scales in this problem and hence, in this specific sense, this is a problem of "Brownian motion."[11] The details of the interactions between the smaller masses of the chain do not affect the dynamics of the heavy impurity which is dictated by λ. For the spin-chain case in the limit of $\alpha\to 0$ a simple minded understanding of the equivalent physics may be as follows. The vanishingly small coupling and hence frequency associated with the nearest-neighbor interactions of the impurity spin may be contrasted with the high-frequency associated with the interactions amongst all the other spins. Again, it is the slowest time scale governed by α that dictates the impurity spin dynamics.

Interestingly, this equivalence between the harmonic oscillator chain and the XY spin chain becomes untenable when α is not vanishingly small. In fact, the dynamics of the impurity spin more closely resembles that of the bulk spin in this regime of α and the problem belongs to a very DUC Ref. 6 under such circumstances. As $\alpha\to 1$, the hypersurface acquires a totally different structure with $\sigma\to(1/4,1/2,3/4,\ldots)$. There is no known example of a problem involving masses connected by harmonic springs that exhibit such a σ.

Quasi-2D attractive quantum fermion gas at T=0 at long wavelengths: The problem with electrons (as fermions) has been extensively studied by many authors.[10] Much progress has been made in constructing exact solution for the dynamics of the density operator in recent years by Lee and Hong.[10] These authors considered the Sawada Hamiltonian[16] and ignored the electron spins to write

$$H=H_0+V, \tag{12}$$

where

$$H_0=\sum_{\vec{k}}\epsilon_k c_{\vec{k}}^\dagger c_{\vec{k}}, \tag{13}$$

$\epsilon_k=k^2/2m$ is the kinetic energy of an electron with momentum $\vec{k}$, $c_{\vec{k}}^\dagger$ ($c_{\vec{k}}$) are creation (annihilation) operators of the fermion with momentum $\vec{k}$, and $V=\Sigma_k\mathscr{V}_k$, where

$$\mathscr{V}_k=\frac{1}{2}v_k\sum_{p\neq p'}{}' [b_{\vec{p}}c_{\vec{p}+\vec{k}}+c_{-\vec{p}-\vec{k}}^\dagger b_{\vec{p}}^\dagger]\sum_{\vec{p}'}{}' [b_{-\vec{p}'}c_{-\vec{p}'-\vec{k}} + c_{-\vec{p}'-\vec{k}}^\dagger b_{-\vec{p}'}^\dagger], \tag{14}$$

where $v_k=2\pi e^2/k$, e=electronic charge, $\hbar\equiv 1$, is the Fourier transform of the Coulomb interaction amongst the spinless electrons in 2D. There is, in general, external pressure/neutralizing background present to stabilize this system. The primes on the sums imply $|\vec{p}|<k_F$, $|\vec{p}+\vec{k}|>k_F$, where k_F is the Fermi momentum and $\vec{p}\neq\vec{p}'$ guarantees that the Pauli exclusion principle is satisfied. The Hamiltonian in Eq. (14) only describes the physics of the particle-hole transitions and ignores the particle-particle (hole-hole) scatterings which also contribute to the total density fluctuations. Knowledge of such density fluctuations readily yields the frequency-dependent polarizibility or the dynamic structure factor.[17]

Let us now focus on the time evolution of this restricted density operator $\tilde{\rho}_{\vec{k}}(t)$ in the sense that the particle-particle (hole-hole) scatterings are ignored,

$$\tilde{\rho}_{\vec{k}}(t)=\sum_{\vec{p}}{}' [d_{\vec{k}}(\vec{p},t)+d_{\vec{k}}^\dagger(-\vec{p},t)], \tag{15}$$

where

$$d_{\vec{k}}(\vec{p},t)\equiv b_{\vec{p}}(t)c_{\vec{p}+\vec{k}}(t), \quad d_{\vec{k}}^\dagger(\vec{p},t)\equiv c_{\vec{p}+\vec{k}}^\dagger(t)b_{\vec{p}}^\dagger(t). \tag{16}$$

This study is valid for high densities and long wavelengths ($k\to 0$) at $T=0$. The calculations reveal that to O(k^2) (Refs. 10,18)

$$\sigma=\left[\frac{nk^2}{m}\left(v_k+\frac{\pi}{m}\right),\epsilon_F^2k^2,\epsilon_F^2k^2,\ldots\right], \tag{17}$$

where $n\equiv k_F^2/2\pi$. Clearly, if the interaction between the fermions is *attractive*, i.e., $v_k=-2\pi e^2/k$ and $2e^2m/k\sim 1$, then σ for this problem becomes identical to the spin-impurity problem in the XY chain at the $\alpha\to 0$ limit and to the heavy impurity problem in the harmonic oscillator chain in the $\lambda\to 0$ limit. This limit for attractive (abnormal) fermions then describes a "Brownian" system in which the dynamics is dictated completely by the slow time scale entering from $(\pi/m-2e^2\pi/k)$.

Physically the fast time scale, entering from $\Delta_n=\epsilon_F^2k^2$ ($n>1$), describes the vibrations of the Fermi surface of the noninteracting system. The slow time scale describes the single-particle excitations corresponding to particle-hole excitations immediately above the Fermi sea due to the attractive interaction between the fermions.

Localization limit: Returning to the XY model, for $\alpha\to\infty$, i.e., a system which effectively behaves as a three spin XY cluster, one finds that the ICF in Eq. (5) truncates at $\Delta_5=0$. This implies that the dynamical behavior is characterized by *three* frequencies at $\omega/\alpha J=0$, $1/\sqrt{2}$ and at $\sqrt{2}$. It turns out that due to the two-dimensional nature of the spin in the XY

model, this behavior is slightly more complex than what one obtains in the $\lambda\to\infty$ limit of the harmonic oscillator chain which simply yields the plasma mode frequency. As pointed out by Lee *et al.*,[5] in the electron-gas problem this corresponds to the case in which the single-particle motions are either frozen or are completely overwhelmed by the plasma oscillation (strong-coupling limit). Thus, for all α except at $\alpha\to 0$, the spin problem is distinct from the other two.

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