Real Time Evolution in Quantum Many-Body Systems With Unitary Perturbation Theory

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We develop a new analytical method for solving real time evolution problems of quantum many-body systems. Our approach is a direct generalization of the well-known canonical perturbation theory for classical systems. Similar to canonical perturbation theory, secular terms are avoided in a systematic expansion and one obtains stable long-time behavior. These general ideas are illustrated by applying them to the spin-boson model and studying its non-equilibrium spin dynamics.

The theoretical investigation of non-equilibrium quantum many-body systems has recently become a very active field of research due to seminal experiments in ultracold atomic gases (for example collapse and revival phenomena [1]), electronic nanostructures (for example transport beyond the linear response regime [2]) and generally qubit dynamics in the presence of quantum dissipation. While non-equilibrium classical systems have been long studied, quantum systems in non-equilibrium hold the promise of many new phenomena yet to be discovered. On the theoretical side, progress is hindered by the notorious difficulty of solving non-equilibrium quantum many-body problems. Motivated by the recent experiments, significant progress has been made with powerful numerical methods like the time-dependent density matrix renormalization group (TD-DMRG) [3] or the time-dependent numerical renormalization group (TD-NRG) [4, 5]. However, there are few reliable analytical methods available, especially for non-perturbative problems (a noteable exeception is the real time RG method [6]).

A key problem for analytical calculations is the appearance of *secular terms* in time t that grow with some power of t. Secular terms appear naturally if one attempts a direct perturbative expansion, e.g. in the Heisenberg equations of motion for the observables. Even if secular terms are multiplied by a small coupling constant, they inevitably invalidate perturbation theory for large times even for small coupling constants and make it impossible to draw conclusions about the long-time behavior. This problem is also very well-known from classical mechanics, dating back to studies of planetary motion in previous centuries. In the context of analytical mechanics, its solution using *canonical perturbation theory* is well-established and can be found in any textbook (see, for example, [7]). The basic idea is to first transform the Hamiltonian to normal form using a canonical transformation. One can then easily solve the equations of motion for the new position and conjugate momentum variables. Only after integrating these equations of motion does one reexpress the old variables in terms of the new time-evolved variables. It is well-established that this yields a much improved long-time solution without any secular terms *even if the canonical transformation itself is only done perturbatively*. Surprisingly, to the best of our knowledge to date no attempt has been made to implement an equivalent scheme based on unitary perturbation theory for quantum many-body systems. However, one key difference to classical systems is that in quantum many-body systems one is often dealing with a continuous energy spectrum, which makes naive unitary perturbation theory impossible due to vanishing energy denominators. A way to solve this specific problem has been established recently by means of the flow equation method [8, 9] (for related ideas see also the similarity renormalization scheme [10]). The central idea of the flow equation method is to diagonalize a many-particle Hamiltonian through a sequence of infinitesimal unitary transformations that eliminate interaction matrix elements with large energy difference first before dealing with smaller energy differences. In this way one both reorganizes a perturbative expansion in an RG-like manner, which allows one to recover non-perturbative energy scales, and one avoids the above small energy denominator problem even for a continuous energy spectrum.

In this Letter we develop the general framework for applying the flow equation method to analytically solve real time evolution problems in quantum many-body systems in exact correspondence to canonical perturbation theory in classical mechanics. We will see that likewise secular terms are avoided and that one can obtain reliable results about the long-time dynamics even in a perturbative framework. We will then illustrate our approach by studying the real time evolution of the spin-boson model with an initially polarized spin and a relaxed bath. The spin-boson model is the paradigm of dissipative quantum systems and its non-equilibrium behavior has recently been investigated using the TD-NRG method [11, 12], which motivates our choice.

Let us briefly review the basic ideas of the flow equation approach (for more details see [9]). A many-body Hamiltonian H is diagonalized through a sequence of infinitesimal unitary transformations with an anti-hermitean generator $\eta(B)$,

$$\frac{dH(B)}{dB} = [\eta(B), H(B)] \ , \tag{1}$$

with $H(B=0)$ the initial Hamiltonian. The "canonical" generator [8] is the commutator of the diagonal part H_0 with the interaction part $H_{\rm int}$ of the Hamiltonian, $\eta(B) \stackrel{\rm def}{=} [H_0(B), H_{\rm int}(B)]$. Under rather general conditions the choice of the canonical generator leads to an increasingly energy-diagonal Hamiltonian $H(B)$, where interaction matrix elements with energy transfer ΔE decay like $\exp(-B\,\Delta E^2)$. For $B=\infty$ the Hamiltonian will be energy-diagonal and we denote parameters and operators in this basis by $\tilde{}$, e.g. $\tilde{H} = H(B=\infty)$.

The key problem of the flow equation approach is generically the generation of higher and higher order interaction terms in (1), which makes it necessary to truncate the scheme in some order of a suitable systematic expansion parameter (usually the running coupling constant). Still, the infinitesimal nature of the approach makes it possible to deal with a continuum of energy scales and to describe non-perturbative effects. This had led to numerous applications of the flow equation method where one utilizes the fact that the Hilbert space is not truncated as opposed to conventional scaling methods. Examples are the evaluation of correlation functions on all energy scales in equilibrium problems [9] and non-equilibrium problems, where one cannot focus on low-energy degrees of freedom anyway (see, for example, the time-dependent Kondo model [13] or the Kondo model with voltage bias [14]).

We will now utilize these features to develop an analogue of canonical perturbation theory in classical mechanics for quantum many-body problems. The general setup is described by the diagram in Fig. 1, where $|\Psi_i\rangle$ is some initial non-thermal state whose time evolution one is interested in. However, instead of following its full time evolution it is more convenient to study the real time evolution of a given observable A. This is done by transforming the observable into the diagonal basis in Fig. 1 (*forward transformation*):

$$\frac{dO(B)}{dB} = [\eta(B), O(B)] \ , \tag{2}$$

with the initial condition $O(B=0) = A$. The central observation is that one can now solve the real time evolution with respect to the energy-diagonal $\tilde{H}$ exactly, thereby avoiding any errors that grow proportional to time (i.e., secular terms): this yields $\tilde{A}(t)$. Now since the initial quantum state is given in the $B=0$ basis, one undoes the basis change by integrating (2) from $B=\infty$ to $B=0$ (*backward transformation*) with the initial condition $O(B=\infty) = \tilde{A}(t)$. One therefore effectively generates a new non-perturbative scheme for solving the Heisenberg equations of motion for an operator, $A(t) = e^{iHt}\,A(0)\,e^{-iHt}$, in exact analogy to canonical perturbation theory. Notice that it is the last step of the backward transformation that distinguishes this scheme from the flow equation evaluation of equilibrium correlation functions [9]: The equilibrium ground state or thermal states are in fact more easily expressed in the $B=\infty$ basis (since $\tilde{H}$ is energy-diagonal) than in the $B=0$ (interacting) basis. It should be mentioned that the same forward-backward transformation scheme with respect to some given initial quantum state has recently also been successfully employed by Cazalilla [16] for studying the nonequilibrium Luttinger model. The main difference to our approach is that the bosonized Luttinger Hamiltonian becomes quadratic, which makes it possible to work out the unitary transformation exactly in [16] (the same holds in [13]): therefore stability questions regarding secular terms for a generic interacting system do not arise, which are the main focus of our work.

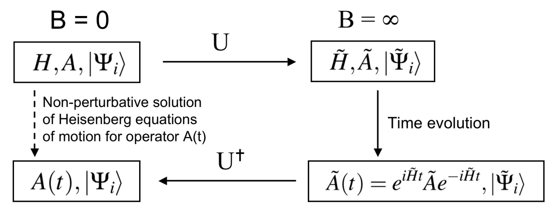

FIG. 1: The forward-backward transformation scheme induces a non-perturbative solution of the Heisenberg equations of motion for an operator. U denotes the full unitary transformation that relates the $B=0$ to the $B=\infty$ basis.[15]

We now illustrate the general idea of our approach by studying the spin-boson model, which serves as a paradigm in dissipative quantum physics and for qubit dynamics (for a review see, for example, [17]):

$$H = -\frac{\Delta}{2}\,\sigma_x + \frac{1}{2}\,\sigma_z\,\sum_k \lambda_k\,(b_k^\dagger + b_k) + \sum_k \omega_k\, b_k^\dagger b_k \ . \tag{3}$$

It describes a two state system coupled to a bath of harmonic oscillators. The effect of this dissipative environment is encoded in the spectral function $J(\omega) \stackrel{\rm def}{=} \sum_k \lambda_k^2\,\delta(\omega - \omega_k)$. In the sequel λ_k is considered a small expansion parameter. In this Letter we will only study the zero temperature case, $T=0$, although the generalization to nonzero temperature is straightforward. We use the following generator for the unitary flow [18]:

$$\begin{aligned}\eta(B) \ &= \ i\,\sigma_y \sum_k \eta_k^{(y)}(b_k + b_k^\dagger) + \sigma_z \sum_k \eta_k^{(z)}(b_k - b_k^\dagger) \\ &\quad + \sum_{k,l} \eta_{kl}\ :(b_k + b_k^\dagger)(b_l - b_l^\dagger): \ ,\end{aligned} \tag{4}$$

with B-dependent coefficients:

$$\eta_k^{(y)} = -\frac{\lambda_k}{2}\,\Delta\,\frac{\omega_k-\Delta}{\omega_k+\Delta}\;, \quad \eta_k^{(z)} = -\frac{\lambda_k}{2}\,\omega_k\,\frac{\omega_k-\Delta}{\omega_k+\Delta}\;,$$
$$\eta_{kl} = \frac{\lambda_k\lambda_l\omega_l\Delta}{2(\omega_k^2-\omega_l^2)}\left(\frac{\omega_k-\Delta}{\omega_k+\Delta}+\frac{\omega_l-\Delta}{\omega_l+\Delta}\right)\;. \qquad (5)$$

Normal-ordering is denoted by : ... :, which serves as a systematic scheme to truncate the infinite sequence of higher and higher operators generated by (1). Higher normal-ordered terms than the ones contained in (3) are neglected in the flow of the Hamiltonian, which amounts to neglecting small (of order λ_k^2) higher order cumulants in the Hamiltonian (this approximation is reliable for any super-Ohmic bath and for an Ohmic bath with $\alpha \lesssim 0.2$, for more details see [9, 18]). If one is interested in equilibrium properties, normal-ordering is performed with respect to the equilibrium ground state, $b_k b_{k'}^\dagger =: b_k b_{k'}^\dagger : +\delta_{kk'}\,n(k)$, where $n(k)$ is the Bose-Einstein distribution. However, later we will be interested in the real time evolution of a non-thermal initial state $|\Psi_i\rangle$. Hence, in order to minimize our truncation error, we write more generally $b_k b_{k'}^\dagger =: b_k b_{k'}^\dagger : +\delta_{kk'}\,n(k) + C_{kk'}$, where $C_{kk'} \stackrel{\text{def}}{=} \langle\Psi_i\,|\,b_k b_{k'}^\dagger\,|\,\Psi_i\rangle - \delta_{kk'}\,n(k)$. The flow of $H(B)$ generated by this η is

$$\frac{d\Delta}{dB} = -\Delta\sum_k \lambda_k^2\,\frac{\omega_k-\Delta}{\omega_k+\Delta} \qquad (6)$$
$$\frac{d\lambda_k}{dB} = -(\omega_k-\Delta)^2\,\lambda_k + 2\sum_l \eta_{kl}\,\lambda_l\;. \qquad (7)$$

The derivation of (6) and (7) is discussed in detail in [9, 18]. The diagonalized Hamiltonian for $B=\infty$ is

$$\tilde{H} = -\frac{\tilde{\Delta}}{2}\,\sigma_x + \sum_k \omega_k\,b_k^\dagger b_k\;, \qquad (8)$$

where $\tilde{\Delta} = \Delta(B=\infty)$ is the renormalized tunneling matrix element. For example for an Ohmic bath, $J(\omega) = 2\,\alpha\,\omega\,\Theta(\omega_c-\omega)$, the renormalized tunneling matrix element derived from the solution of the flow equations [9, 18] has the correct non-perturbative behavior [17], $\tilde{\Delta} \propto \Delta\,(\Delta/\omega_c)^{\alpha/1-\alpha}$.

The observables in the $B=\infty$ basis are given by solving (2) for a suitable ansatz for the flowing observable [9]. For example,

$$\sigma_x(B) = h(B)\,\sigma_x + \sigma_z\sum_k\Big(\chi_k(B)\,b_k + \bar{\chi}_k(B)\,b_k^\dagger\Big)$$
$$+\; \alpha(B) + i\sigma_y\sum_k\Big(\mu_k(B)\,b_k - \bar{\mu}_k(B)\,b_k^\dagger\Big) \qquad (9)$$

where higher normal-ordered terms generated in $O(\lambda_k^2)$ during the flow (2) are again neglected. The differential

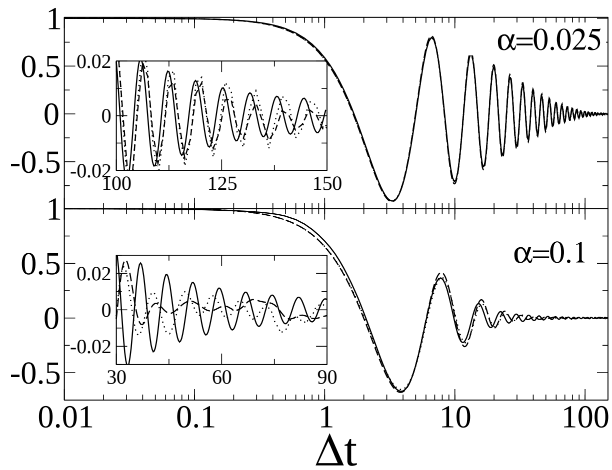

FIG. 2: Real time evolution of the spin expectation value $\langle\sigma_z(t)\rangle$ starting from a polarized spin in z-direction with a relaxed Ohmic bath (see text) for two different values of α and $\omega_c/\Delta = 10$. The full lines are the flow equation results, the dashed lines TD-NRG curves for $\Lambda = 2.0$ and the dotted lines for $\Lambda = 1.41$. The TD-NRG results are courtesy of F. Anders, see [11]. The various curves agree extremely well except for very long times shown in the insets.

equations describing this flow take the following form:

$$\frac{dh}{dB} = -\sum_k\Big(\eta_k^{(y)}(\chi_k+\bar{\chi}_k) + \eta_k^{(z)}(\mu_k+\bar{\mu}_k)\Big)$$
$$-4\sum_{k,l}\eta_k^{(y)}\,C_{kl}(\chi_l+\bar{\chi}_l)$$
$$\frac{d\chi_k}{dB} = 2\,h\,\eta_k^{(y)} + \sum_l\Big(\eta_{kl}(\chi_l+\bar{\chi}_l) + \eta_{lk}(\bar{\chi}_l-\chi_l)\Big)$$
$$\frac{d\mu_k}{dB} = 2\,h\,\eta_k^{(z)} - \sum_l\Big(\eta_{lk}(\mu_l+\bar{\mu}_l) + \eta_{kl}(\mu_l-\bar{\mu}_l)\Big)$$
$$\frac{d\alpha}{dB} = \sum_k\Big(\eta_k^{(y)}(\mu_k+\bar{\mu}_k) + \eta_k^{(z)}(\chi_k+\bar{\chi}_k)\Big)\;, \qquad (10)$$

with the initial conditions $h(B=0)=1, \chi_k(B=0) = \mu_k(B=0) = \alpha(B=0) = 0$. For $\Delta \in \operatorname{supp} J(\omega)$ the observable decays completely, $\tilde{h} \stackrel{\text{def}}{=} h(B=\infty) = 0$, implying decoherence [9]. The ground state expectation value of σ_x is then given by $\tilde{\alpha} \stackrel{\text{def}}{=} \alpha(B=\infty)$.

For real time evolution problems we now solve the Heisenberg equations of motion in the diagonal basis, $\tilde{\sigma}_z(t) = e^{i\tilde{H}t}\tilde{\sigma}_z e^{-i\tilde{H}t}$. The result is straightforward

$$\tilde{\chi}_k(t) = \big(\tilde{\chi}_k(0)\cos(\tilde{\Delta}t) + i\,\tilde{\mu}_k(0)\sin(\tilde{\Delta}t)\big)e^{-i\omega_k t} \qquad (11)$$
$$\tilde{\mu}_k(t) = \big(\tilde{\mu}_k(0)\cos(\tilde{\Delta}t) + i\,\tilde{\chi}_k(0)\sin(\tilde{\Delta}t)\big)e^{-i\omega_k t}\;,$$

while $\tilde{h}$ and $\tilde{\alpha}$ remain unchanged. In complete analogy to canonical perturbation theory, we next undo the unitary transformation (2). The values of $\tilde{h}, \tilde{\alpha}, \tilde{\chi}_k(t), \tilde{\mu}_k(t)$ are used as initial values in the system of differential equa-

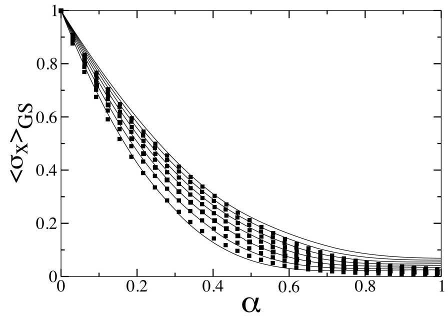

FIG. 3: Ground state expectation value of σ_x: Comparison of flow equation results (curves) and NRG data (squares) from [19] for an Ohmic bath with damping α. The results are for $\omega_c/\Delta = 25, 28.6, 33.3, 40, 50, 66.7, 100$ from top to bottom.

tions (10) at $B = \infty$, which is then integrated backwards to $B = 0$. This yields $h(t), \alpha(t), \chi_k(t), \mu_k(t)$, which parametrize the time-evolved operator σ_x,

$$\sigma_x(t) \;=\; h(t)\,\sigma_x + \sigma_z \sum_k \Big(\chi_k(t)\,b_k + \bar{\chi}_k(t)\,b_k^\dagger\Big) \\ +\;\; \alpha(t) + i\sigma_y \sum_k \Big(\mu_k(t)\,b_k - \bar{\mu}_k(t)\,b_k^\dagger\Big) \qquad (12)$$

in the original basis of the problem. Thereby the forward-backward transformation scheme induces a non-perturbative solution of the Heisenberg equations of motion, compare Fig. 1.

For the purposes of this Letter, we focus on the numerical solution of the above differential equations by discretizing the bosonic bath with $O(10^3)$ modes (notice that an approximate analytical treatment is equally possible). The initial quantum state $|\Psi_i\rangle$ is taken as spin up, $\langle\Psi_i|\sigma_z|\Psi_i\rangle = +1$, with a relaxed bath with respect to this fixed spin. This yields $C_{kk'} = \lambda_k\lambda_{k'}/4\omega_k\omega_{k'}$. We have implemented the numerical solution for all components of the spin degree of freedom. In order to assess the accuracy of our approach, the time evolution of $\langle\sigma_z(t)$ is shown in Fig. 2 and compared with TD-NRG data for two values of the discretization parameter Λ. One finds excellent agreement except for very long time scales (shown in the insets of Fig. 2), where the TD-NRG discretization error becomes noticeable (since the curves depend on Λ). The flow equation solution for the observable $\langle\sigma_x(t)\rangle$ shows that it approaches its flow equation equilibrium expectation value $\langle\sigma_x\rangle_{\rm GS}$ with an absolute error below 10^{-2} for long times. A comparison of $\langle\sigma_x\rangle_{\rm GS}$ with exact numerical results using NRG [19] in Fig. 3 again shows very good agreement.

Summing up, we have shown how to implement an analogous scheme to canonical perturbation theory for quantum many-body systems. Using a simple but non-trivial example, we could demonstrate that the well-established advantages of canonical perturbation theory versus naive perturbation theory carry over to our unitary perturbation approach as well, in particular the absence of secular terms in real time evolution problems. Our results are stable in the long-time limit (see Figs. 2,3) and can be improved systematically in a *uniform* manner (as a function of time) by higher orders of the calculation. The underlying scheme of infinitesimal unitary transformations permits to study non-perturbative effects [20]. Similar to the role of canonical perturbation theory in analytical mechanics, our approach should be useful for other real time evolution problems from impurity systems to lattice models in quantum many-body physics [21].

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