# Collective versus Single–Particle Motion in Quantum Many–Body Systems: Spreading and its Semiclassical Interpretation

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We study the interplay between collective and incoherent single–particle motion in a model of two chains of particles whose interaction comprises a non–integrable part. In the perturbative regime, but for a general form of the interaction, we calculate the spectral density for collective excitations. We obtain the remarkable result that it always has a unique semiclassical interpretation. We show this by a proper renormalization procedure which allows us to map our system to a Caldeira–Leggett–type of model in which the bath is part of the system.

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Collective motion, *i.e.*, coherent motion of the particles in phase space, is a fundamental feature of many–body systems. A wealth of information on collectivity is available for atomic nuclei [1]. Bose–Einstein condensates [2–4] provide more recent examples. There is strong experimental [5] and theoretical [6] evidence that similar effects occur in other fermionic systems as well. Collective motion emerges out of the incoherent, single–particle motion whenever favored by energy and kinematic conditions. Due to the quantum–classical correspondence principle, the collective dynamics on the classical level should be reflected in the spectral properties of the corresponding quantum many–body system. Hence, the spectrum of a many–body system comprises states of single–particle and of collective character, mixed forms with a partial degree of collectivity exist as well. The details strongly depend on how the system is probed.

Consider the Giant Dipole Resonance in heavier nuclei as a prominent example which also serves as an inspiration for our model to be discussed in the sequel. The cross section of electric dipole radiation and the spectral density of the excitations show at a certain energy a huge peak whose spreading width is orders of magnitudes larger than the mean level spacing. It can be understood in terms of the following picture: the neutrons are confined to one sphere, the protons to another one. There is no or very little relative motion of the nucleons inside these spheres. The two spheres, however, move against each other, resulting in an enormous response function. The difference between the center–of–mass coordinates of the two spheres is the proper collective coordinate. Many other forms of collective motion in nuclei exist.

Not surprisingly, it is a demanding challenge to understand the emergence of collective motion and its interplay with the incoherent single–particle motion. The vast majority of studies in this context relies on effective models whose justification is often mainly phenomenological or even on the level of hand waving if the system in question is too complex. Better understanding of these issues is called for. In the present contribution, we have three goals: (i) We want to address the interplay between collective and single–particle motion from first principles in the framework of a tractable, yet sufficiently general and complex model. (ii) We aim at doing this analytically in such a way that we identify the collective coordinate, but always keep full control over the single–particle degrees of freedom. (iii) We wish to deliver the important insight that the spectral density of the collective excitations is directly related to classical motion.

We begin with setting up our model which considerably generalizes an integrable model which we studied previously [7]. In one dimension, two chains $a = 1, 2$ of $N$ interacting particles each with positions $x_i^{(a)},\ i = 1, \ldots, N$ and momenta $p_i^{(a)},\ i = 1, \ldots, N$ are coupled to one another. The total Hamiltonian reads

$$H = H_0 + \lambda H_1 \ . \tag{1}$$

Here, $H_0 = H_0^{(1)} + H_0^{(2)} + H_0^{(12)}$ is the integrable part considered in Ref. [7]. The first two terms

$$H_0^{(a)} = \frac{1}{2m} \sum_{i=1}^{N} \left( p_i^{(a)} \right)^2 + \sum_{i,j=1}^{N} x_i^{(a)} W_{ij} x_j^{(a)} \tag{2}$$

model the two chains $a = 1, 2$ before they are coupled. The interaction within each chain is harmonic and described by the matrix $W$ which we assume equal in both chains. We are mainly interested in selfbound systems such as nuclei, where unlike Bose–Einstein condensates no external confining potential is needed. It is easy to impose corresponding conditions on the matrix $W$ which ensure that the interaction is invariant under translations and the system is bounded [7]. We now couple the two chains by an interaction which depends on the differences between their coordinates,

$$H_0^{(12)} = \sum_{i,j=1}^{N} K_{ij} \left( x_i^{(1)} - x_j^{(2)} \right)^2 \ . \tag{3}$$

For every choice of the coupling matrix $K$, the Hamiltonian $H_0$ is translation invariant. Clearly, the model is up to now integrable.

We generalize the model by adding the translation invariant term $\lambda H_1$ which breaks integrability,

$$H_1 = \sum_{i,j=1}^{N} f(x_i^{(1)} - x_j^{(2)}) \ , \tag{4}$$

where $f$ is an arbitrary, positive and even analytical function of the form

$$f(z) = \sum_{n=2}^{\infty} f_n z^{2n} \ . \tag{5}$$

We introduce the parameter $\lambda$, because we aim at a perturbative discussion.

To quantize our model, we replace coordinates and momenta by operators $\hat{x}_i^{(a)}$ and $\hat{p}_i^{(a)}$. Importantly, we make this step on the level of the *original* particle degrees of freedom. Motivated by the above mentioned Giant Dipole Resonance, we aim at studying collective excitations and the associated spectral density. We expect that it shows a pronounced peak, which we wish to understand in (semi)classical terms. Naturally, the collective coordinate $X$ is the difference between the mass centers of the two chains, and it is convenient to rescale it with a factor $\sqrt{N/2}$,

$$X = \frac{1}{\sqrt{2N}} \left( \sum_{i=1}^{N} x_i^{(1)} - \sum_{i=1}^{N} x_i^{(2)} \right) \tag{6}$$

and accordingly for the collective operator $\hat{X}$. To probe the existence of quantum collective states in the excitation spectrum, we investigate the correlator

$$S(t) = \langle \Phi_0 | \hat{X}(t) \hat{X}(0) | \Phi_0 \rangle \ , \tag{7}$$

where $|\Phi_0\rangle$ is the ground state of the total Hamiltonian $\hat{H}$. Here, $\hat{X}(t)$ is the Heisenberg picture of the operator $\hat{X}$ with the time evolution governed by the total Hamiltonian $\hat{H}$. The Fourier transform of the correlator (7),

$$\tilde{S}(\omega) = \sum_{\mu=0}^{\infty} |\langle \Phi_0 | \hat{X} | \Phi_\mu \rangle|^2 \delta \left( \omega - \frac{E_\mu - E_0}{\hbar} \right) \ , \tag{8}$$

is the desired spectral density of the collective excitations. It measures the strength of the transitions between the ground and the excited states $|\Phi_\mu\rangle$ of the whole system and can be interpreted as the response of the system that is excited by the transition operator $\hat{X}$. Following the terminology in many–body physics, we say that there is a collective quantum state for an energy $E_{\rm col} = E_0 + \hbar\omega$ if $\tilde{S}(\omega)$ (smoothened over some energy interval) has a pronounced spike at the corresponding frequency $\omega$.

To leading order $\lambda$ in perturbation theory, we obtain the following expression for the correlator

$$\begin{aligned} S(t) &\approx \langle 0 | \hat{X}_I(t) \hat{X}_I(0) | 0 \rangle \\ &+ \lambda \sum_{l \neq 0} \left( a_{l0}^1 \langle 0 | \hat{X}_I(t) \hat{X}_I(0) | l \rangle + (a_{l0}^1)^* \langle l | \hat{X}_I(t) \hat{X}_I(0) | 0 \rangle \right) \\ &+ \frac{i\lambda}{\hbar} \int_0^t dt_1 \langle 0 | [H_I(t_1), \hat{X}_I(t)] \hat{X}_I(0) | 0 \rangle + \mathcal{O}(\lambda^2) \ , \end{aligned} \tag{9}$$

where the sum runs over the eigenstates $|l\rangle$ of $\hat{H}_0$, and where $|0\rangle$ is the ground state of $\hat{H}_0$. The coefficients $a_{l0}^1 = \langle l | \hat{H}_1 | 0 \rangle / (E_0 - E_l)$ turn out to be real due to time reversal invariance. The sum in Eq. (9) arises from the correction to the ground state while the last term results from the perturbation of the Hamiltonian. The collective operator $\hat{X}_I$ and the non–integrable part $\hat{H}_{1I}$ of the Hamiltonian appear in the interaction picture whose time evolution is governed by the integrable Hamiltonian $\hat{H}_0$. For any operator $\hat{F}$, we have

$$\hat{F}_I(t) = \exp\left( \frac{i}{\hbar} \hat{H}_0 t \right) \hat{F} \exp\left( -\frac{i}{\hbar} \hat{H}_0 t \right) \ . \tag{10}$$

For later purposes, it is useful to consider the imaginary part of the correlator, ${\rm Im} S(t) = S_1(t)$. We notice that, by virtue of Eq. (8), the Fourier transforms of $S(t)$ and $S_1(t)$ are connected through

$$\tilde{S}(\omega) = 2i\Theta(\omega) \tilde{S}_1(\omega) \ , \tag{11}$$

where $\Theta(\omega)$ denotes the Heaviside step function. Since ${\rm Im}\langle 0 | \hat{X}_I(t) \hat{X}_I(0) | l \rangle$ vanishes for $l \neq 0$, the imaginary part of the correlator simplifies, and we find

$$\begin{aligned} S_1(t) &\approx {\rm Im} \langle 0 | \hat{X}_I(t) \hat{X}_I(0) | 0 \rangle \\ &+ \frac{\lambda}{2\hbar} \int_0^t dt_1 \langle 0 | \left[ [\hat{H}_{1I}(t_1), \hat{X}_I(t)], \hat{X}_I(0) \right] | 0 \rangle + \mathcal{O}(\lambda^2) \ . \end{aligned} \tag{12}$$

At this point, we may use our previous results [7]. The first term of Eq. (12) was evaluated by mapping $H_0$ into the form of a Caldeira–Leggett–like model, in which $X$ can be viewed as the coordinate of a "big" particle in a harmonic potential which is coupled to a "bath" of harmonic oscillators. The interpretation of the "bath", however, differs significantly form the standard Caldeira–Leggett situation [8]. In our case, the "bath" is not external, it is part of the system and formed by the internal degrees of freedom. The resulting expression for the spectral function $\tilde{S}(\omega)$ is then

$$\tilde{S}(\omega) \approx \frac{\hbar}{\pi m} \Theta(\omega) \ {\rm Im} \frac{1}{\Omega_0^2 - \omega^2 - i\omega\tilde{\gamma}(\omega)} \ , \tag{13}$$

where $\tilde{\gamma}$ formally coincides with the classical "damping" kernel, but here it describes the spreading of the collective excitation over the spectrum. There is not an energy loss or any kind of dissipation in our system. The resonance frequency $\bar{\Omega}_0$ is the fundamental oscillator frequency of the corresponding classical problem. To illustrate this result, we mention that, when the collective degree of freedom $X$ interacts with an ohmic "bath" (see Ref. [9]), the spreading kernel $\tilde{\gamma}(\omega) = \gamma_0$ is a constant and $\tilde{S}(\omega)$ has a Lorentzian shape with the width $\gamma_0$ at the position of the classical oscillator frequency $\bar{\Omega}_0 = \sqrt{\Omega_0^2 - (\gamma_0/2)^2}$.

We now consider the crucial second term on the right hand side of Eq. (12). A naive continuation of the approach in Ref. [7] quickly becomes cumbersome. Luckily, there is much better way of tackling this term which eventually leads to a new insight to our problem. The second term is easily seen to be of the form $\frac{\lambda}{2\hbar}\int_0^t dt_1 \chi(t_1,t)$, with the kernel $\chi(t_1,t)$ given by

$$\sum_{i\neq j}\langle 0|\left[[f(\hat{x}_i^{(1)}(t_1) - \hat{x}_j^{(2)}(t_1)), \hat{X}(t)], \hat{X}(0)\right]|0\rangle \ . \quad (14)$$

Owing to the harmonic form of $\hat{H}_0$, we find the identity

$$[(\hat{x}_i^{(1)} - \hat{x}_j^{(2)})^n, \hat{X}(-t)] = n(\hat{x}_i^{(1)} - \hat{x}_j^{(2)})^{n-1}\beta_{ij}(t) \quad (15)$$

for the commutator of the $n$–th powers of differences with the collective operator. For all $n$, it can be reduced to the operator $(\hat{x}_i^{(1)} - \hat{x}_j^{(2)})^{n-1}$ multiplying the function $\beta_{ij}(t)$ defined by $[(\hat{x}_i^{(1)} - \hat{x}_j^{(2)}), \hat{X}(-t)] = \beta_{ij}(t)\mathbf{1}$. We notice that the commutator in the latter expression is proportional to the unit operator $\mathbf{1}$. Applying this formula twice yields

$$\chi(t_1,t) = \beta_{ij}(t_1 - t)\beta_{ij}(t_1)C_{ij} \ , \quad (16)$$

where the elements of the matrix $C$ are given by the ground state expectation values involving the second derivative of the arbitrary function $f$ defining the non–integrable part of the interaction in Eq. (4),

$$C_{ij} = \langle 0|f''(\hat{x}_i^{(1)} - \hat{x}_j^{(2)})|0\rangle \ . \quad (17)$$

We emphasize that this result is not due to an expansion of the function $f(z)$, it applies in leading order $\lambda$ to all functions of the form (5).

We arrive at the important insight anticipated above: precisely the same equation for the kernel $\chi(t_1,t)$ follows when using the harmonic Hamiltonian

$$\hat{H}_0^{\mathrm{R}} = \hat{H}_0 + \frac{\lambda}{2}\sum_{i,j=1}^{N} C_{ij}(\hat{x}_i^{(1)} - \hat{x}_j^{(2)})^2 \ . \quad (18)$$

In other words, the effect of a general, non–integrable perturbation can, to leading order $\lambda$, be fully accounted for by a proper renormalization of the integrable Hamiltonian $\hat{H}_0$. Since $\hat{H}_0^{\mathrm{R}}$ is harmonic, the spectral function $\tilde{S}(\omega)$ is given by Eq. (13), where the renormalized oscillation frequency $\Omega_0^{\mathrm{R}}$ and the spreading kernel $\gamma^{\mathrm{R}}$ depend on the constant matrix elements $C_{ij}$.

The $C_{ij}$ themselves depend on the parameters of the integrable Hamiltonian $\hat{H}_0$. Starting from the definition (17), we derive

$$C_{ij} = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} f''(x\sqrt{\alpha_{ij}})\exp\left(-\frac{x^2}{2}\right)dx \ , \quad (19)$$

where the quantities $\alpha_{ij} = \langle 0|(x_i^{(1)} - x_j^{(2)})^2|0\rangle$ can be related to the parameters of $\hat{H}_0$. They are given by $\alpha_{ij} = (\Gamma_{ii} + \Gamma_{jj})/4$, where $\Gamma_{kk}$ is the $k$-th diagonal element of the matrix

$$\Gamma = \frac{\hbar}{\sqrt{2m}}\left(\left(\frac{1}{W+M-K}\right)^{1/2} + \left(\frac{1}{W+M+K}\right)^{1/2}\right) \ , \quad (20)$$

and $M$ is a diagonal matrix whose elements read [7] $M_{ij} = \delta_{ij}\sum_l K_{il}$. The coefficients $C_{ij}$ depend on $\hbar$ since they result from sandwiching the function $f$ with the ground states of the integrable Hamiltonian. If we restrict ourselves to leading order $\hbar$, only the first term of the expansion (5) enters. In such a semiclassical regime Eq. (19) simplifies and we have $C_{ij} = 3f_2(\Gamma_{ii} + \Gamma_{jj})$.

Since $H_0^{\mathrm{R}}$ is harmonic, the spectral function $\tilde{S}(\omega)$ can now be calculated using Eq. (13). The renormalized oscillator frequency $\Omega_0^{\mathrm{R}}$ and the renormalized spreading kernel $\gamma^{\mathrm{R}}$ are determined by the renormalized coupling constants $K_{ij}^{\mathrm{R}} = K_{ij} + \lambda C_{ij}/2$ and by $W_{ij}$. The spreading kernel can be expressed through the spectral density function $\sigma^{\mathrm{R}}(\omega)$ [9],

$$\gamma^{\mathrm{R}}(t) = \frac{2}{m}\int_0^{\infty}\frac{\sigma^{\mathrm{R}}(\omega)}{\omega}\cos(\omega t)d\omega \ . \quad (21)$$

Employing our previous results [7], we express the spectral density function through the parameters of the harmonic Hamiltonian. This yields

$$\sigma^{\mathrm{R}}(\omega) = -\frac{1}{2\pi m\omega}\mathrm{Im}\,\mathbf{k}^T\frac{\mathbb{1}}{(\omega + i\epsilon)\mathbb{1} - (2K_r/m)^{1/2}}\mathbf{k}, \quad (22)$$

where $K_r$ and $\mathbf{k}$ are obtained from the matrix $\tilde{K}^{\mathrm{R}} = A^T(W + M^{\mathrm{R}} + K^{\mathrm{R}})A$, with $A$ being a discrete $N \times N$ cosine transform (DCT), see Ref. [7]. More precisely, $K_r$ is the $(N-1)\times(N-1)$ matrix obtained from $\tilde{K}^{\mathrm{R}}$ by deleting the first row and the first column while the vector $\mathbf{k}$ is the first column (excluding the first element) of $\tilde{K}^{\mathrm{R}}$. The renormalized oscillator frequency turns out to be

$$\Omega_0^{\mathrm{R}} = \sqrt{2\tilde{K}_{11}^{\mathrm{R}}/m + \gamma^{\mathrm{R}}(0)} \ . \quad (23)$$

It is important to notice that the spreading kernel (21), the oscillator frequency (23) and therefore the spectral density $\tilde{S}(\omega)$ are fully determined by the *classical* dynamics of the renormalized Hamiltonian $\hat{H}_0^{\mathrm{R}}$. In particular, using our previous results [7], the equation for the classical time evolution of the collective coordinate reads

$$\frac{d^2X(t)}{dt^2} + (\Omega_0^{\rm R})^2 X(t) + \int_0^t \gamma^{\rm R}(t-s)\frac{dX(s)}{ds}ds = 0 \ . \quad (24)$$

The same equation holds for the expectation value $\langle\hat{X}\rangle(t)$ if the initial state of the system is properly chosen. Equation (24) describes a damped, *i.e.* in our case spread, harmonic oscillator whose spreading kernel $\gamma^{\rm R}(t)$ and oscillator frequency $\Omega_0^{\rm R}$ are given by Eqs. (21) and (23), respectively. Importantly, the solution of Eq. (24) also determines, for properly chosen initial conditions, the spectral density of the collective excitations. We notice, however, that $\hat{H}_0^{\rm R}$ itself contains quantum corrections which depend on $\hbar$. Put differently, $\hat{H}_0^{\rm R}$ is identified as the proper effective Hamiltonian whose classical dynamics — rather than the classical dynamics of the original, total Hamiltonian $\hat{H}$ — determines the spectrum of collective excitations in leading order $\lambda$. We also notice that higher order terms in the perturbative treatment of $S(t)$ come with higher powers of $\hbar$. Indeed, it is straightforward to see that in the case of $f(z) = f_2 z^4$ the $n$–th term of the perturbative expansion scales as $(\hbar\lambda)^n$. In this sense the renormalized Hamiltonian $\hat{H}_0^{\rm R}$ provides the first semiclassical correction to the spectrum of the collective modes.

We briefly discuss the conditions for the validity of our perturbative approach. The approximation (9) can be used if the following conditions are satisfied, see Ref. [10]. First, the gap between the ground state and the first excited state of $\hat{H}_0$ must be sufficiently large, i.e., $\lambda|\langle 0|\hat{H}_1|0\rangle| \ll \hbar\omega_{\rm min}$, where $\omega_{\rm min}$ is the minimal oscillator frequency of the classical system given by the lowest eigenvalue of the matrix $W + M + K$. Second, the time $t$ of propagation must be bounded by $\lambda|\langle 0|\hat{H}_1|0\rangle|t/\hbar \ll 1$. As we are interested in time scales of order $t \sim \Omega_0^{-1}$, the first condition implies the second one. Under these conditions the spectral characteristics such as energy and spreading width of the collective excitations are close to their values for the unperturbed Hamiltonian $\hat{H}_0$. We notice, however, that such a "small" perturbation $\lambda H_1$ might be quite large on the scale of the mean level spacing which is of the order $\hbar^N$. This means that the local distribution of the energy levels of the Hamiltonian $H$ might be essentially different from the energy level distribution of the integrable Hamiltonian $H_0$.

In conclusion, we studied, in the framework of a simple model, the emergence of collectivity from first principles. We did not start from an effective model, we rather derived an effective description and still kept full control over the original degrees of freedom. In doing so, we relate the expectation value of the collective operator and the spectral density of the collective excitations to a purely *classical* equation. We consider that to be important, as it can be viewed as a justification of the routinely used strategy in many–body physics, where effective models are set up classically and then quantized.

Beside the fundamental aspects just mentioned, there is further motivation for our study: Statistical analysis of the spectra indicates that collective motion is typically regular while the incoherent single–particle motion yields spectral statistics described by random matrices, see Refs. [11–13]. This coexistence of both regular and chaotic dynamics in the same system is a truly intriguing dynamical aspect of many–body systems [14]. The regularity of collective motion implies that the recent arguments [15] strongly supporting the Bohigas–Giannoni–Schmit conjecture for single–particle systems do not carry over in a straightforward manner to many–body systems. In short, this conjecture states that the spectral statistics of the single–particle system is of random–matrix type if the corresponding classical system is chaotic. Our study is thus needed when addressing the role of collectivity in quantum chaos.

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