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Concepts in Many-Body Systems Illustrated by Coupled Oscillators*

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The system of coupled oscillators forms a very simple many-body system that can be treated exactly within elementary quantum mechanics. This system is used to introduce important many-body concepts, such as spectral function, propagator or Green function, sum rule, and elementary excitation. These concepts are briefly discussed for the real system of conduction electrons interacting with lattice vibrations.

A MODEL SYSTEM

It is the purpose of this article to present a problem which presupposes nothing but the most elementary quantum mechanics and still illustrates in a simple fashion some important ideas and concepts for many-body systems. One of the key problems in this branch of physics is the following: Suppose that we have added a particle with momentum \mathbf{p}_1 to a many-body system at time t_1 . What is the probability of finding the particle with momentum \mathbf{p}_2 at time t_2 ? For non-interacting particles the probability will be unity for $\mathbf{p}_1 = \mathbf{p}_2$ and zero otherwise.¹ For interacting particles the probability will be a number between

zero and one that depends on the state of all the other particles at time t_1 . Further, if the particles are identical, i.e., indistinguishable, we must ask for the probability of finding *any* particle with momentum \mathbf{p}_2 at time t_2 .

As an illustration we will consider a very simple many-body system consisting of two interacting oscillators with unequal masses m_1 and m_2 , force constants k_1 and k_2 , and a coupling constant k_3 . We then have the Hamiltonian

$$H = p_1^2/(2m_1) + p_2^2/(2m_2) + \frac{1}{2}k_1x_1^2 + \frac{1}{2}k_2x_2^2 + \frac{1}{2}k_3(x_1 - x_2)^2, \quad (1)$$

where p_1 and p_2 are momenta and x_1 and x_2 position coordinates for the oscillators. If $k_3 = 0$, we say that the system consists of two (unequal) independent oscillators, 1 and 2 (in many-body jargon, "bare" oscillators). The corresponding wave functions are $\Phi_n(x_1)$ and $\chi_m(x_2)$. When $k_3 \neq 0$, a simple transformation (see Appendix) will give us the Hamiltonian of two uncoupled displaced oscillators (primed wave functions, new oscillator frequencies ω_1' , ω_2' , and energy eigenvalues E_{nm}'). Let us now consider one single oscillator in its ground state. We add to this system another "bare" oscillator in its N th excited state and switch on instantaneously an interaction according to Eq. (1). In other words, we have at time $t=0$ a wave function $\psi_{0,N}(t=0) = \Phi_0(x_1)\chi_N(x_2)$. This is not an eigenstate of the Hamiltonian (1). To find the evolution in time, we therefore make an expansion in the complete set of wave functions Φ' and χ' for the transformed uncoupled oscillators:

$$\psi_{0,N}(t) = \sum_{m,n} A_{m,n}{}^{0,N} \Phi_m' \chi_n' \times \exp\{-i[(m + \frac{1}{2})\omega_1' + (n + \frac{1}{2})\omega_2']t\}. \quad (2)$$

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The expansion coefficients are related in a recursive way (see Appendix).

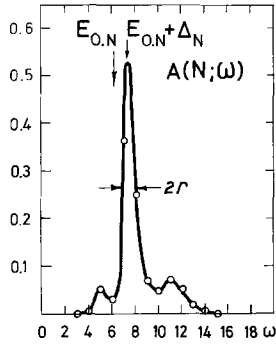


FIG. 1. The spectral function $A(N; \omega)$ for $N=7$ bare excited state. The force constants are $k_1=k_2=1$, $k_3=0.7$. The masses have been so chosen that the frequency ratio is $\omega_1'/\omega_2'=2$; ω_2' is taken as the energy unit. The arrow points at the energy of $E_{0,N}$ of the bare states. The half width 2Γ and the energy shift Δ_N are also shown.

Let us define a *spectral function* $A(N; \omega)$:

$$A(N; \omega) = \sum_{m,n} |A_{m,n}{}^{0,N}|^2 \delta(E_{mn}' - \hbar\omega). \quad (3)$$

The integral,

$$\int_{\omega_0}^{\omega_0+\Delta\omega} A(N; \omega) d(\hbar\omega), \quad (4)$$

gives the probability that a measurement of the excitation energy yields a result which lies in the interval $[\hbar\omega_0, \hbar(\omega_0+\Delta\omega)]$. All wave functions are normalized to unity, i.e.,

$$1 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} |\psi_{0,N}|^2 dx_1 dx_2 = \sum_{m,n} |A_{m,n}{}^{0,N}|^2. \quad (5)$$

Thus, we find that the spectral function obeys a *sum rule*:

$$\int A(N; \omega) d(\hbar\omega) = 1. \quad (6)$$

As an illustration, we have calculated numerically the spectral function for a particular choice of parameters in Eq. (1) (Fig. 1). A smooth curve has been drawn through the discrete set of delta function amplitudes. A Lorentzian shaped curve A' (not shown in the figure) can be fitted to the main peak of $A(N; \omega)$; A' can be written

$$A'(N; \omega) = (z_N/\pi) \Gamma_N / [(\hbar\omega - E_{0,N} - \Delta_N)^2 + \Gamma_N^2]. \quad (7)$$

It is easy to see that A' would contribute the fraction z_N to the sum rule (6).

We next ask for the probability that a system which is initially in the bare state $\psi_{0,N}$ will still be found there at time t . It is easy to verify that this probability is the squared norm of a probability amplitude $G(N; t)$ which can be written as the Fourier transform

$$G(N; t) = \int_{-\infty}^{\infty} A(N; \omega) \exp(-i\omega t) d(\hbar\omega). \quad (8)$$

This expression follows immediately from the well-known form in elementary quantum mechanics for the probability amplitude, namely

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \psi_{0,N}^*(t) \psi_{0,N}(0) dx_1 dx_2. \quad (9)$$

$G(N; t)$ contains information about the evolution of the system both in space and time and is often referred to as a *propagator function*. It corresponds closely to the ordinary Green functions of many-body systems.^{2,3} From Eq. (8) we see that the information contained in the propagator function is also in the spectral function, and we can use either expression as a starting point for interpretations.

INTERPRETATION

Our model calculation can be given an interpretation that brings us close to many concepts in real many-body systems. We started with the introduction of one "bare" oscillator in its N th excited state. This oscillator was allowed to interact with a many-body system in its ground state, which in our simple case happens to consist of only one particle (i.e., the other oscillator). If it were not for this interaction, the first oscillator would remain in its N th eigenstate forever and the spectral function would be just one single delta function:

$$A(N; \omega) = \delta(E_{0,N} - \hbar\omega). \quad (10)$$

With interactions, the system will have a complicated evolution in time that is mathematically described by the full spectral function. From Fig. 1 we see that $A(N; \omega)$ has a fairly sharp peak of width 2Γ superposed on a more or less irregular

background. The main peak corresponds to a wave packet with terms in Eq. (2) that stay *approximately coherent* (i.e., they all have the same phase) over a time $\tau = \hbar/2\Gamma$. The other terms in Eq. (2) corresponding to the irregular background in the spectral function will get out of phase in a time much shorter than τ and add up approximately to zero. Therefore, for times $t < \tau$ (but not too small), the wave packet takes the approximate form

$$\psi_{0,N}(t) \approx \Phi(x_1, x_2) \exp[-i(E_{0,N} + \Delta_N)t/\hbar], \quad (11)$$

where $\Phi(x_1, x_2)$ is a function of the coordinates x_1 and x_2 only. If τ is long compared to the period of oscillation of the right-hand side of Eq. (11), this expression can be considered as an approximate eigenstate. It can be labeled by the quantum numbers $(0, N)$ of the bare state and has a time dependence similar to that of a true eigenstate. On the other hand, the wave function in Eq. (11) is not normalized to unity. The system is described as containing an *elementary excitation* with quantum number $(0, N)$, strength z_N , life time $\hbar/2\Gamma$, and energy shifted from the “bare” value $E_{0,N}$ to $E_{0,N} + \Delta_N$. It is only when the spectral function has a pronounced peak that it has any meaning to talk about elementary excitations. Figure 2 shows how $A(N; \omega)$ changes with excitation energy. For higher N values, the spectral function can no longer be given a simple interpretation in terms of elementary excitations. A more detailed account of the interpretation given here can be found, e.g., in Ref. 2.

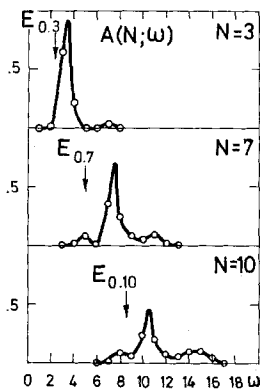


FIG. 2. The spectral function $A(N; \omega)$ for three bare excited states ($N=3, 7, 10$). Parameters as in Fig. 1.

REAL SYSTEM

We will now see what form the concepts introduced above will take in a real many-body system.⁴ We choose as an example the interaction between the electron gas and the lattice vibrations in an almost ideal metal. Thus, for simplicity we consider zero temperature and neglect electron-electron interaction as well as band effects due to the periodicity of the lattice. A free “bare” electron of momentum \mathbf{p} is supposed to be injected into the system. Inside the metal, the bare electron is no longer in an eigenstate because of the interaction with the lattice vibrations. Following the idea of our model calculation for the harmonic oscillators, we could try to expand the wave function for the bare electron in terms of eigenstates for the interacting case. As momentum is conserved, it is natural to label the excited interacting system by \mathbf{p} . If there were no coupling between the injected electron and the lattice vibrations, the system would be described by a spectral function that is a delta function:

$$A(\mathbf{p}, \omega) = \delta[(p^2/2m - E_F) - \hbar\omega]. \quad (12)$$

It is natural to describe the excitation energies relative to the Fermi energy E_F since no electrons can be injected into states of lower energy because of the Pauli principle. With interactions included, the spectral function may still have a pronounced peak of width smaller than the excitation energy. The corresponding elementary excitation constitutes what is called a *quasi particle*. It carries a momentum \mathbf{p} but has an energy-momentum relation that is different from $E_p = p^2/2m - E_F$. In Fig. 3 we plot the spectral function for a real system (sodium). The electron state has a momentum \mathbf{p} . Without interactions with phonons the energy is $E = p^2/2m$. With interactions the state can still be assigned a momentum \mathbf{p} , but there is a shift and a spread in the energy which is given by the spectral function. The Fermi energy is at $\omega=0$. The curve is from a calculation by Grimvall (see Ref. 5) using a realistic form of the electron-phonon interaction.

One of the virtues of the many-body theory as presented above is that many of the results valid for a system of non-interacting particles can be retained for the interacting system if only we

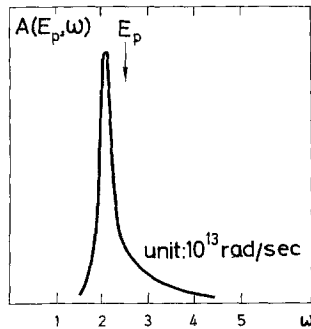


FIG. 3. The spectral function for a real system—electrons interacting with phonons in sodium at $T=0$ K. The Fermi energy is at $\omega=0$ and $E_p=p^2/2m-E_F$ is the bare energy, i.e., without any electron-phonon interactions. The curve is from a calculation by Grimvall (see Ref. 5).

think in terms of quasi particles instead of bare particles. As an example we can consider the heat capacity of an electron gas, a quantity that does not depend on the wave function but only on the density of states. For electrons interacting with the lattice vibrations we get mathematically the same result as for the non-interacting case, if only we replace the bare-electron density of states at the Fermi level by the quasi-particle density of states. Thus, important properties of many-body systems may be treated in an approximate way in terms of elementary excitations without recourse to the exact spectral function. The spectral function (or the propagator) will completely describe the interacting system [see Eq. (2)]. Therefore, even if the quasi-particle picture is not valid, we can find, e.g., the thermodynamic properties from expressions involving an integration over the spectral function.⁵ As a last practical example, we note that the quasi particle decays after a time τ . In other words, we can say that the injected electron has a lifetime τ before it is scattered, and therefore the mean free path is $\mathbf{p}\tau/m$. There are several other examples from solid state theory where we can apply the concepts introduced. Not only electrons but also photons may interact with the lattice vibrations. This gives rise to elementary excitations called polaritons.⁶ As another example, we note that the lattice vibrations (phonons) in a real crystal are never strictly harmonic but are coupled via anharmonic interactions. Consequently, the form of the spectral function will deviate from a delta

function.⁷ As a last example, we can mention that in an electron gas, the plasma oscillations couple to the individual electrons and give rise to an electron spectral function with considerable structure.⁸

SUMMARY

A complete description of a many-body system requires full knowledge of the wave function. In general, the wave function contains too much information; in many cases it is enough to find the distribution of excitation energies. That information is conveniently obtained from a spectral function or, alternatively, its Fourier transform (Green function). The spectral function may have a sharp peak superposed on an irregular background. The peak corresponds to an elementary excitation, and its width is inversely proportional to the life time of the excitation. These concepts were introduced for a simple model system consisting of two coupled oscillators and then discussed for the real systems of electrons in metals interacting with the lattice vibrations.

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APPENDIX

A transformation to normal modes is accomplished by a simple change of coordinates:

$$\begin{aligned} x_1' &= x_1 \cos\alpha - (m_2/m_1)^{1/2}x_2 \sin\alpha, \\ x_2' &= x_1 \sin\alpha + (m_2/m_1)^{1/2}x_2 \cos\alpha. \end{aligned} \tag{A1}$$

The original Hamiltonian transforms to that of two uncoupled oscillators if

$$\tan(2\alpha) = \frac{2k_3(m_1/m_2)^{1/2}}{k_1+k_3 - (m_1/m_2)(k_2+k_3)}. \tag{A2}$$

Elementary quantum mechanics gives us the expansion coefficients A_{nm}^{0N} as

$$A_{mn}^{0N} = \iint \psi_{0N}^*(x_1, x_2) \Phi_m'(x_1') \chi_n'(x_2') dx_1 dx_2. \tag{A3}$$

The eigenfunctions of a harmonic oscillator that enter the integrand of Eq. (A3) have the form of an exponential times a Hermite polynomial. Using the recursive relations⁹

$$\begin{aligned} 2zH_n &= H_{n+1} + 2nH_{n-1}, \\ dH_n/dz &= 2nH_{n-1}, \end{aligned} \quad (A4)$$

for the Hermite polynomials $H_n(z)$, one finds that the expansion coefficients A_{mn}^N ($A_{mn}^{0N} = A_{mn}^N$) can be related in a recursive way, Eqs. (A5) and (A6). The calculations are lengthy but straightforward, and we only give the final results:

$$\begin{aligned} A_{00}^0 &= 2(h_1 h_2 k_1 k_2 m_1 m_2^3)^{1/8} / c \\ A_{10}^1 &= 4(h_1 h_2 k_1 k_2 m_1 m_2^3)^{1/8} b_1 b_3 / (c \sigma_4) \\ A_{01}^1 &= 4(h_1 h_2 k_1 k_2 m_1 m_2^3)^{1/8} b_2 b_3 / (c \sigma_4) \quad (A5) \\ A_{mn}^N &= (2a_1^2/\sigma_1 + 2b_1^2/\sigma_4 - 1) [(m-1)/m]^{1/2} A_{m-2,n}^N \\ &\quad + 2(a_1 a_2/\sigma_1 + b_1 b_2/\sigma_4) (n/m)^{1/2} A_{m-1,n-1}^N \\ &\quad + 2b_1 b_3/\sigma_4 (N/m)^{1/2} A_{m-1,n}^{N-1} \\ A_{mn}^N &= 2(a_1 a_2/\sigma_1 + b_1 b_2/\sigma_4) (m/n)^{1/2} A_{m-1,n-1}^N \\ &\quad + (2a_2^2/\sigma_1 + 2b_2^2/\sigma_4 - 1) [(n-1)/n]^{1/2} A_{m,n-2}^N \\ &\quad + 2b_2 b_3/\sigma_4 (N/n)^{1/2} A_{m,n-1}^{N-1} \\ A_{mn}^N &= 2b_1 b_3/\sigma_4 (m/N)^{1/2} A_{m-1,n}^{N-1} \\ &\quad + 2(b_2 b_3/\sigma_4) (n/N)^{1/2} A_{m,n-1}^{N-1} \\ &\quad + (2b_3^2/\sigma_4 - 1) [(N-1)/N]^{1/2} A_{mn}^{N-2}. \quad (A6) \end{aligned}$$

¹ In some cases, e.g., the free electron model for metals, the particle interaction is approximated by a constant potential. Such a model retains the properties of an independent particle system. An analogous situation is the use of hydrogen-like wave functions in many electron atoms.

² P. Nozières, *Theory of Interacting Fermi Systems* (Benjamin, New York, 1963), pp. 58-73.

³ J. R. Schrieffer, *Theory of Superconductivity* (Benjamin, New York, 1964), Chaps. 5, 6; in particular pp. 112-114, 158-161.

⁴ Throughout this paper we consider distinguishable particles in our model problem, and therefore some important aspects of real many-body systems are left out. If we had two identical particles that were fermions (i.e., obeying the Pauli principle), the wave function of their

$A_{mn}^N = 0$ if any $N, m, n < 0$ or if $N+m+n$ is odd. This set of recursive equations is easily solved on a computer. In Eqs. (A5) and (A6) we have for brevity used the following symbols:

$$\begin{aligned} h_1 &= (k_1 + k_3) \cos^2 \alpha + (m_1/m_2) (k_2 + k_3) \\ &\quad \times \sin^2 \alpha + k_3 (m_1/m_2)^{1/2} \sin 2\alpha \\ h_2 &= (k_1 + k_3) \sin^2 \alpha + (m_1/m_2) (k_2 + k_3) \\ &\quad \times \cos^2 \alpha - k_3 (m_1/m_2)^{1/2} \sin 2\alpha \\ a_1 &= (h_1 m_1/\hbar^2)^{1/4} \cos \alpha \\ a_2 &= (h_2 m_1/\hbar^2)^{1/4} \sin \alpha \\ \beta_1 &= (h_1 m_2^2/\hbar^2 m_1)^{1/4} \sin \alpha \\ \beta_2 &= (h_2 m_2^2/\hbar^2 m_1)^{1/4} \cos \alpha \\ \gamma_1 &= (k_1 m_1/\hbar^2)^{1/4} \\ \gamma_2 &= (k_2 m_2/\hbar^2)^{1/4} \\ \sigma_1 &= a_1^2 + a_2^2 + \gamma_1^2 \\ \sigma_2 &= \beta_1^2 + \beta_2^2 + \gamma_2^2 \\ \sigma_3 &= -a_1 \beta_1 + a_2 \beta_2 \\ \sigma_4 &= \sigma_2 - (\sigma_3^2/\sigma_1) \\ b_1 &= -\beta_1 - a_1 (\sigma_3/\sigma_1) \\ b_2 &= \beta_2 - a_2 (\sigma_3/\sigma_1) \\ b_3 &= \gamma_2 \\ c &= \hbar (\sigma_1 \sigma_4)^{1/2} \end{aligned}$$

ground state may have components that correspond to the N th excited bare state of one particle. Therefore it would not be possible with probability 1 to add a third identical particle in the N th bare state. We have not found it worth while to carry out an analysis of three coupled oscillators that would illustrate a many-body system of identical particles.

⁵ G. Grimvall, *Phys. kondens. Materie* **9**, 283 (1969).

⁶ C. Kittel, *Quantum Theory of Solids* (Wiley, New York, 1963), pp. 42-44.

⁷ R. A. Cowley, *Rept. Prog. Phys.* **31**, 123 (1968).

⁸ L. Hedin and S. Lundqvist, *Solid State Phys.* **23**, 1 (1969), in particular pp. 86-87.

⁹ L. I. Schiff, *Quantum Mechanics* (McGraw-Hill, New York, 1955), p. 63.