EXCITATION SPECTRUM OF A PARTICLE SYSTEM IN AN EXTERNAL FIELD

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A set of equations defining the excitation spectrum and decay of the initial individual excitation is derived from the linearized Hartree equations by taking the initial conditions into account. The quantum dispersion relation and its classical analog, which specify the collective excitation spectrum of a system in an external field, are deduced.

A linear approximation of the Hartree self-consistent field method has been used many times to determine the spectrum of collective and single-particle excitations of systems of interacting particles.[1,2] A consistent application of this method should obviously include the formulation and solution of the initial-condition problem (the Cauchy problem). In the present paper we show that for a given approximation Heitler's formalism[3] not only yields the spectrum of the collective and single-particle excitations of the system in an external field, but determines the decay of an initial individual or collective state.

We consider a system of interacting particles in an external field. The operator equation for the density matrix, in a representation determined by the eigenvalues of the particle states in the external field, has the form

$$\{i\hbar\,\partial/\partial t - E_n + E_{n'}\}\,\rho\,(nn') = \sum_{ll'}\Big\{\rho\,(ll')\,\rho\,(mm')\,G^{nl'}_{ml}\,\delta\,(n'm') - \rho\,(mm')\,\rho\,(ll')\,G^{m'l'}_{n'l}\,\delta\,(nm)\Big\} \equiv \sum_{ll'} G^{nl'}_{n'l}\{\rho(ll')\,\rho\,(n'n') - \rho\,(nn)\,\rho\,(ll')\} + \Delta\rho(nn'); \quad (1)$$

$$G^{nl'}_{n'l} = \int dx\,dy\,G\,(x-y)\,\psi^{+}_{n}(x)\,\psi^{+}_{l'}(y)\,\psi_{n'}(x)\,\psi_{l}(y). \quad (1')$$

Here $G(x-y)$ is the kernel of the interaction between particles, and $\psi_l(x)$ satisfies the equation

$$\{T\,(p) + U\,(x)\}\,\psi_l(x) = E_l\psi_l\,(x).$$

Averaging the operator equation for the density matrix over the state of the system (in the occupation-number space) and using further the Hartree approximation in which the diagonal elements of the averaged density matrix are replaced by the distribution functions of the non-interacting particles in the external field:

$$\langle\rho\,(ll')\,\rho\,(nn)\rangle \to \langle\rho\,(ll')\rangle\langle\rho\,(nn)\rangle \to f\,(E_n)\,\langle\rho\,(ll')\rangle,$$

we obtain in the linear approximation $\langle\Delta\delta\,(nn')\rangle \to 0$, i.e., a system of Hartree equations, which is a natural generalization of the system considered by Ehrenreich and Cohen[2]

$$\{i\hbar\,\partial/\partial t - E_n + E_{n'}\}\,\langle\rho\,(nn')\rangle = \Delta f\,(nn')\sum_{ll'} G^{nl'}_{n'l}\langle\rho\,(ll')\rangle,$$
$$\Delta f\,(nn') = f(E_{n'}) - f(E_n). \quad (2)$$

We assume that in the system of linearlized Hartree equations the self action of the particles has been eliminated, so that

$$\sum_{ll'} G^{nl'}_{n'l}\langle\rho\,(ll')\rangle \to \sum_{ll' \neq nn'} G^{nl'}_{n'l}\langle\rho\,(ll')\rangle.$$

We proceed to analyze the Hartree system with allowance for an initial condition in the form

$$\langle\rho\,(n_0n_0')\rangle_{t\to 0^+} = 1,\quad \langle\rho\,(nn')\rangle_{t\leqslant 0} = 0,\qquad nn' \neq n_0n_0'.$$

Using the expansion

$$\langle\rho\,(nn')\rangle = \frac{1}{2\pi i}\int dE\,\rho_{nn'|n_0n_0'}(E)\,\exp\,[-iEt/\hbar],$$

we find that allowance for the initial condition leads to the system

$$D_{nn'}(E)\,\rho_{nn'|n_0n_0'}(E) = \Delta f\,(nn')\sum_{ll'} G^{nl'}_{n'l}\,\rho_{ll'|n_0n_0'}(E) + \delta\,(n_0n_0'\,|\,nn'),$$
$$D_{nn'}(E) = E - E_n + E_{n'}. \quad (3)$$

Following Heitler's formalism[3] we introduce for $ll' \neq n_0n_0'$ a new matrix, defined by the relation

$$\rho_{ll'|n_0n_0'}(E) = U_{ll'|n_0n_0'}(E)\,D^{-1}_{ll'}(E)\,\rho_{n_0n_0'|n_0n_0'}(E),$$

$$D^{-1}_{nn'}(E) = \mathrm{P}\,[E - E_n + E_{n'}]^{-1} - i\pi\delta\,(E - E_n + E_{n'}).$$

The system of homogeneous equations

$$U_{nn'|n_0n_0'}(E) = \Delta f\,(nn')\sum_{ll'} G^{nl'}_{n'l} D^{-1}_{ll'}(E)\,U_{ll'|n_0n_0'}(E) \quad (4)$$

determines the introduced matrix for $nn' \neq n_0n_0'$, and the relation

$$\rho_{n_0n_0'|n_0n_0'}(E) = [D_{n_0n_0'}(E) + \frac{i}{2}\Gamma_{n_0n_0'}(E)]^{-1}, \qquad (5)$$

$$\frac{1}{2}\Gamma_{n_0n_0'}(E) = i\Delta f(n_0n_0')\sum_{ll'} G_{n_0l}^{n_0l'} D_{ll'}^{-1}(E)\, U_{ll'|n_0n_0'}(E) \qquad (6)$$

determines the behavior of the initial condition.

The quantity $\Gamma_{n_0n_0'}(E)$ is, generally speaking, complex and determines the line width of the single-particle transition $n_0' \to n_0$ and the energy shift of the single-particle transition. We note that $\Gamma_{n_0n_0'}(E)$ vanishes when $n_0' = n_0$, corresponding to the absence of a shift and to the natural width of the single-particle level.

To separate the spectrum of the collective fluctuations, we parametrize the resultant system of equations. Actually, expanding the interaction kernel in the expression for the matrix element of the transition $G_{n'l}^{nl'}$ in a Fourier series

$$G_{n'l}^{nl'} = \sum_q G(q)\,(n\,|e^{iqx}|\,n')\,(l'\,|e^{iqx}|\,l),$$

and introducing the generalized collective operator

$$U_q(E;\; n_0n_0') = \sum_{ll'} (l'|e^{iqx}\,|\,l)\, D_{ll'}^{-1}(E)\, U_{ll'|n_0n_0'}(E), \qquad (7)$$

we find that the width and the shift of the energy of the single-particle transition are expressed in terms of the introduced quantity as follows:

$$\frac{1}{2}\Gamma_{n_0n_0'}(E) = i\Delta f(n_0n_0')\sum_q G(q)\,(n_0\,|e^{iqx}|\,n_0')\,U_q(E;\; n_0n_0'). \qquad (8)$$

By simple transformation of the system of homogeneous equations for $U_{nn'|n_0n_0'}$ we find that the collective operator $U_q(E;\, n_0n_0')$ should satisfy the equation

$$\{1 - G(q)\sum_{nn'}\Delta f(nn')D_{nn'}^{-1}(E)\,|(n\,|e^{iqx}|\,n')|^2\}\, U_q(E;\; n_0n_0')$$
$$= \sum_{q'\neq q} G(q')\, U_{q'}(E;\; n_0n_0')$$
$$\times \sum_{nn'} \Delta f(nn')\, D_{nn'}^{-1}(E)\;\; (n\,|e^{iq'x}|\,n')\,(n'\,|e^{iqx}|\,n), \qquad (9)$$

the structure of which is such as to permit the separation

$$U_q(E;\; n_0n_0') = U_q(E)\; U(n_0n_0'),$$

which leads to the possibility of existence of a collective-excitation spectrum $E(q)$ independent of the quantum numbers of the individual initial condition. This last circumstance is again a consequence of the elimination of terms corresponding to the self-action of the particles from the initial Hartree equations.

Neglecting the right half in the complete system (9), we arrive to a quantum dispersion relation in closed form

$$1 = G(q)\sum_{nn'} \mathrm{P}\frac{f(E_{n'}) - f(E_n)}{E - E_n + E_{n'}}\,|(n\,|e^{iqx}|\,n')|^2$$
$$- i\pi G(q)\sum_{nn'} \delta(E - E_n + E_{n'})$$
$$\times [f(E_{n'}) - f(E_n)]\,|(n\,|e^{iqx}|\,n')|^2, \qquad (10)$$

solution of which determines the spectrum of the collective fluctuations of the system of interacting particles.

Relation (5) together with the expression (8) determines the energy shift and the line width of the initial individual excitation of the system in the presence of collective excitation with a spectrum defined by the dispersion relation (10). To find the classical analog of the dispersion relation (10), we change in this expression from summation over (n, n') to summation over $(n, \Delta n = n' - n)$ and take account of the fact that in the classical approximation the main contribution is due to the eigenvalues $n \gg \Delta n \gg 1$. Since the quasi-classical matrix elements approach zero rapidly with increasing Δn and change little with changing n when the difference Δn is fixed, we use, on going to the classical dispersion relation, the expansion

$$E - E_{n+\Delta n} + E_n \to E - (\partial E_n/\partial n)\,\Delta n = E - \hbar\omega(n)\,\Delta n,$$
$$f(E_{n+\Delta n}) - f(E_n) \to (\partial f(E_n)/\partial E_n)\,\hbar\omega(n)\,\Delta n,$$

where, according to reference 4,

$$\omega(n) = \partial E_n/\partial I, \qquad I = \frac{1}{2\pi}\oint p\,dx.$$

In addition, it is necessary to take account of the fact that the matrix element of the transition goes in the classical limiting case into the corresponding Fourier component of a function defined on the classical trajectory of the particle. After simple transformations we obtain a classical analog of the dispersion relation (10)

$$1 = G(q)\sum_{n,\,\Delta n} \mathrm{P}\frac{\hbar\omega(n)\,\Delta n}{E - \hbar\omega(n)\,\Delta n}\frac{\partial f(E_n)}{\partial E_n}\left|\int dt\, e^{iqx(t) - i\omega(n)\Delta n t}\right|^2$$
$$- i\pi G(q)\sum_{n,\,\Delta n}\delta(E - \hbar\omega(n)\,\Delta n)$$
$$\times \frac{\partial f(E_n)}{\partial E_n}\hbar\omega(n)\,\Delta n\left|\int dt\, e^{iqx(t) - i\omega(n)\Delta n t}\right|^2, \qquad (10')$$

where $x(t)$ is a solution of the classical problem of the motion of a particle in an external field.

The dispersion relations (10) and (10′) obtained above lead, in the case of infinitesimally small wave numbers ($q \to 0$), to generalized Lorentz dispersion sums. For particles that are free in the ground state the complete system of equations for the collective operator coincides identically with the cut-off system and (10) goes into the well known Klimontovich-Silin dispersion equation.[1] We note that the Hartree-Fock approximation leads in this situation to a system that determines a collective operator analogous to the complete system (9).

For a system in a periodic field, in the approximation

$$(n, \mathbf{k}\,|\,e^{i\mathbf{qr}}\,|\,\mathbf{k}',\ n') \to (u_{\mathbf{k},n}\,|\,u_{\mathbf{k+q},n'})\,\delta\,(\mathbf{k}'-\mathbf{k}-\mathbf{q}),$$

where $(n, \mathbf{k}\,|\,\mathbf{r}) \equiv u_{\mathbf{k}},\ n(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}$ defines the state of a particle with quasi-momentum $\mathbf{k}$ in band n, corresponding to conservation of the quasi-momentum in the single-particle transition $\mathbf{k}'$, n' $\to$ $\mathbf{k}$, n, the dispersion relation (10) goes into the dispersion equation of the band model.[2] Finally, for a system of particles in a constant homogeneous magnetic field, in the approximation

$$(k_x,\ n,\ k_z\,|\,e^{i\mathbf{qr}}\,|\,k_z',n',k_x')$$
$$\to \delta\,(k_z'-k_z-q_z)\,\delta\,(k_x'-k_x-q_x)\,(\chi_n\,|\,\chi_{n'})\,\delta\,(q_y),$$

where $(\chi_n\,|\,\chi_{n'})$ is the overlap integral of the oscillator functions, corresponding to the Landau representation,[4] we arrive at the dispersion equation obtained by Zyryanov.[5]

Let us turn now to an examination of the "collective" initial condition, which is an assembly of initial conditions with definite wave number values

$$R_q(0) = \sum_{n_0 n_0'} (n_0\,|\,e^{iqx}\,|\,n_0')\,\rho^{(0)}(n_0 n_0'). \tag{11}$$

Parametrizing relation (5), which determines the behavior of each individual initial condition, we find that the quantity

$$R_q(E) = \sum_{n_0 n_0'} (n_0\,|\,e^{iqx}\,|\,n_0')\,\rho_{n_0 n_0'\,|\,n_0 n_0'}(E), \tag{12}$$

which characterizes the behavior of the assembly of initial conditions with definite wave number values, is determined by the relation

$$R_q(E) = \sum_{n_0 n_0'} \frac{(n_0\,|\,e^{iqx}\,|\,n_0')}{D_{n_0 n_0'}(E) + i\Gamma_{n_0 n_0'}(E)/2}\,\rho^{(0)}(n_0 n_0'). \tag{13}$$

Relation (13) in general does not lend itself to separation in the right-hand part of the 'collective' initial condition. However, in the approximation $\langle D^{-1}\rangle_{av} = \langle D\rangle_{av}^{-1} + \ldots$ we find that

$$R_q(E) = [D_q(E) + i\Gamma_q(E)/2]^{-1} R_q(0), \tag{14}$$

where the fluctuation propagation function

$$D_q(E) = \sum_{n_0 n_0'} D_{n_0 n_0'}(E)\,(n_0\,|\,e^{iqx}\,|\,n_0')\,\rho^{(0)}(n_0 n_0')$$

is the propagation function of the single-particle transition averaged over the initial state, and the decay of the fluctuations is determined by the averaged width

$$\tfrac{1}{2}\Gamma_q(E) = iG(q)F(q,\ q)\,U_q(E) + i\sum_{q'\neq q} G(q')\,F(q,\ q')\,U_{q'}(E),$$

$$F(q,\ q') = \sum_{n_0 n_0'} \Delta f\,(n_0 n_0')\,(n\,|\,e^{iq'x}\,|\,n_0')\,(n_0'\,|\,e^{iqx}\,|\,n_0)\,\rho^{(0)}(n_0 n_0').$$

In conclusion we note that parametrization of the initial Hartree equations leads in the presence of self-action to a system of inhomogeneous equations for the collective operator $U_q(E;\ n_0 n_0')$, of the form

$$U_q(E;\ n_0 n_0') = \{1 - G(q)\sum_{nn'} \Delta f(nn')\,D_{nn'}^{-1}(E)\,|\,(n\,|\,e^{iqx}|n')|^2\}^{-1}$$
$$\times \Big\{\sum_{nn'} \Delta f\,(nn')\,D_{nn'}^{-1}\,(E)\,(n\,|\,e^{iqx}\,|\,n')\,G^{n_0' n}_{n_0 n'} + \sum_{q'\neq q} G(q')\,U_{q'}(E;\ n_0 n_0')$$
$$\times \sum_{nn'} \Delta f(nn')\,D_{nn'}^{-1}(E)\,(n\,|\,e^{iq'x}\,|\,n')\,(n'\,|\,e^{iqx}\,|\,n)\Big\}. \tag{15}$$

In this case the state of collective fluctuations of the system is determined not only by the excitation spectrum $E = E(q)$, but by the quantum numbers of the initial individual excitation $(n_0,\ n_0')$. The system given above for the definition of $U_q(E;\ n_0 n_0')$, together with the expression for $\rho_{n_0 n_0'\,|\,n_0 n'}(E)$, analogous to that given above, determines the decay of the initial individual state and the excitation of collective fluctuations in the system of interacting particles.

For particles that are free in the ground state the equation for the collective operator $U_q(E;\ k_0,\ k_0')$ is greatly simplified and turns into the analog of the following equation[1]

$$\rho_{\mathbf{k}}(t) = \frac{1}{2\pi i}\oint ds e^{st} \times \Big\{1 - G(k)\int \frac{f(\mathbf{p}+\hbar\mathbf{k}/2) - f(\mathbf{p}-\hbar\mathbf{k}/2)}{m^{-1}kp - is}\,d^3p\Big\}^{-1} \times \int \frac{\varphi_{\mathbf{k}}(0,\mathbf{p})}{s + im^{-1}\mathbf{kp}}\,d^3p,$$

which determines the time variation of the Fourier component of the density fluctuation $\rho_{\mathbf{k}}(t)$ in terms of the initial value of the perturbed particle distribution function of the system, $\varphi_{\mathbf{k}}(0,\ \mathbf{p})$.

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[1] Yu. L. Klimontovich and V. P. Silin, Usp. Fiz. Nauk **70**, 247 (1960), Soviet Phys.-Uspekhi **3**, 84 (1960).

[2]H. Ehrenrich and M. H. Cohen, Phys. Rev. **115**, 786 (1959).

[3]W. Heitler. The Quantum Theory of Radiation, Oxford 1954.

[4] L. D. Landau and E. M. Lifshitz, Quantum Mechanics, I. Pergamon, 1948.

[5]P. S. Zyryanov, JETP **40**, 1065 (1961), this issue p. **751**.

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