WAVE EQUATION OF PARTICLE DENSITY OPERATOR

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The problem of wave equation which describes phonons in a many-particle system is considered.

Starting from

$$\rho(\vec{r},t) = \sum_i \delta(\vec{r} - \vec{r}_i(t)) \quad , \tag{1}$$

$$\rho(\vec{r},t) = \sum_{\vec{k}} \rho_{\vec{k}} e^{i\vec{k}\vec{r}} = \frac{1}{L^3} \sum_{i,\vec{k}} e^{-i\vec{k}\vec{r}_i + i\vec{k}\vec{r}} \tag{2}$$

and assuming two-body interaction,

$$H = \sum_i \frac{p_i^2}{2m} + \frac{1}{2} \sum_{i,j}{}' V_{ij} \tag{3}$$

follows

$$\frac{\partial^2 \rho}{\partial t^2} = -\frac{1}{L^3} \frac{1}{4m^2} \sum_{i,\vec{k}} \left(e^{-i\vec{k}\vec{r}_i} (\vec{k}\vec{p}_i)^2 + 2\vec{k}\vec{p}_i e^{-i\vec{k}\vec{r}_i} \vec{k}\vec{p}_i + (\vec{k}\vec{p}_i)^2 e^{-i\vec{k}\vec{r}_i} \right) e^{i\vec{k}\vec{r}} +$$

$$+ \frac{1}{L^3} \frac{i}{m} \sum_{i,\vec{k}} (\vec{k}\nabla_i V) e^{-i\vec{k}\vec{r}_i} \cdot e^{i\vec{k}\vec{r}} \tag{4}$$

Let be $\{|n\rangle\}$ complete set of eigenvectors of the Hamiltonian (3). The operator $\sum_{i,\vec{k}} e^{-i\vec{k}\vec{r}_i} (\vec{k}\vec{p}_i)^2$ with respect to basis of these vectors reads

$$\langle n | \sum_{i,\vec{k}} e^{-i\vec{k}\vec{r}_i} (\vec{k}\vec{p}_i) | m \rangle = \sum_{i,\vec{k}} e^{\frac{i}{\hbar}(E_n - E_m)t} \langle n | \{ e^{-i\vec{k}\vec{r}_i} (\vec{k}\vec{p}_i) \}_{t=0} | m \rangle \quad . \tag{5}$$

Assumption (1):

$$\langle \vec{r}_1 \dots \vec{r}_N | m \rangle \equiv \Psi_m = e^{\chi} \varphi_m (\vec{r}_1 \dots \vec{r}_N) \; . \tag{6}$$

This assumption gives

$$(\vec{k}\vec{p}_i)^2 \Psi_m = \varphi_m (\vec{k}\vec{p}_i)^2 e^{\chi} + e^{\chi} (\vec{k}\vec{p}_i)^2 \varphi_m + 2(-i\hbar)^2 (\vec{k}\nabla_i) e^{\chi} (\vec{k}\nabla_i) \varphi_m \cdot \tag{7}$$

Assumption (2): The last two terms on the right side can be neglected for each m.

Eq.(7) can be then written in the form

$$(\vec{k}\hat{\vec{p}}_i)^2\psi_m = \varphi_m\, \zeta_{\vec{k}i} = \varphi_m \Big(\sum_j{}' \zeta^{(1)}_{\vec{k}}(\vec{r}_{ij}) + \sum_{jj'}{}' \zeta^{(2)}_{\vec{k}}(\vec{r}_{ij},\vec{r}_{ij'}) + \cdots \Big). \tag{8}$$

Assumption (3):

$$\sum_{j(\neq i)} \rightarrow \frac{1}{\Omega_0} \int_{\text{non } \Omega_0} d\vec{r}_j \tag{9}$$

where Ω_0 is the average volume per particle. This assumption leads to

$$\zeta_{\vec{k}i} = \frac{1}{\Omega_0} \int_{\text{non } \Omega_0} \zeta^{(1)}_{\vec{k}}(\vec{\varrho})\, d\vec{\varrho} + \cdots \equiv k^2 \zeta . \tag{10}$$

By making use of $\Delta e^{i\vec{k}\vec{r}} = -k^2 e^{i\vec{k}\vec{r}}$, one gets

$$\frac{1}{L^3} \sum_{i,\vec{k}} e^{-i\vec{k}\vec{r}_i} (\vec{k}\hat{\vec{p}}_i)^2 e^{i\vec{k}\vec{r}} = -\zeta \Delta \varrho . \tag{11}$$

Application of the same procedure on each term of Eq.(4) gives

$$\frac{\partial^2 \varrho}{\partial t^2} = \Big(\frac{\zeta}{m^2} + w_2 \Big) \Delta \varrho + \Big(-\frac{\hbar^2}{4m} + w_4 \Big) \Delta^2 \varrho + \cdots \tag{12}$$

where

$$w_2 = -\frac{1}{m} \frac{4\pi}{3} \frac{1}{\Omega_0} \int_{\text{non } \Omega_0} \varrho^3 \frac{dV_{12}}{d\varrho} d\varrho , \tag{13}$$

$$w_4 = -\frac{1}{m} \frac{2\pi}{15} \frac{1}{\Omega_0} \int_{\text{non } \Omega_0} \varrho^5 \frac{dV_{12}}{d\varrho} d\varrho . \tag{14}$$

Retaining only the second order space changes one gets

$$\Delta \varrho - \frac{1}{v^2} \frac{\partial^2 \varrho}{\partial t^2} = 0 \tag{15}$$

where is

$$v^2 = \frac{\zeta}{m^2} + w_2 . \tag{16}$$

This is desirable equation.

The application of this equation to the liquid He^4 with the Morse-like potential which is determined from the Yntema-Schneider potential [1]

$$V_{12}(r) = a\, e^{-\alpha r} - b\, e^{-\beta r} \tag{17}$$

gives for the sound velocity v=662 m/sec. The experimental value is 240 m/sec. A better evaluation of the sum in (9) in which short-range correlative motions are included gives v=379 m/sec.

References

[1] J.L.Yntema,W.G.Schneider, J.Chem.Phys. 18,(1950) 641.

"Bose Condensation in the System of Frenkel Excitons and Optical P operties of the Exciton Condensate"

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As it was shown in /1/, where the collective properties of Frenkel excitons were studied in details, the Hamiltonian of the exciton system, in the presence of the condensate, has (in the Bogoliubov's approximation) the following form: $H = \sum_{\vec{k}\neq 0}\left(\frac{\hbar^2 k^2}{2m} + \frac{4\pi\hbar^2 f N_0}{mV}\right)B^+_{\vec{k}}B_{\vec{k}} +$

$$+ \frac{2\pi\hbar^2 f N_0}{mV}\sum_{\vec{k}\neq 0}\left(B^+_{\vec{k}}B^+_{-\vec{k}} + B_{-\vec{k}}B_{\vec{k}}\right). \qquad (1)$$

Here $\frac{\hbar^2 k^2}{2m}$ -is the exciton energy in the effective mass approximation and calculated from the "bottom" of the exciton zone, $f=\frac{a}{2}$ is the scattering length for exciton scattering on the δ-potential and $\frac{N_0}{V}$-the exciton concentration.

The system of equations of motion for the Green's functions: $\langle\langle B_{\vec{k}}(t)|B^+_{\vec{k}}(0)\rangle\rangle$ and $\langle\langle B^+_{-\vec{k}}(t)|B^+_{\vec{k}}(0)\rangle\rangle$, obtained from the Hamiltonian (1), gives the single-particle Green function (in energy representation at $T=0$):

$$\langle\langle B_{\vec{k}}|B^+_{\vec{k}}\rangle\rangle_E = \frac{1}{2\pi}\left[\frac{N_{\vec{k}}+1}{E-\mathcal{E}(\vec{k})+i\delta} - \frac{N_{\vec{k}}}{E+\mathcal{E}(\vec{k})+i\delta}\right]. \qquad (2)$$

The pole of this function gives the energy of elementary excitations:

$$\mathcal{E}(\vec{k}) = \left[\left(\frac{\hbar^2 k^2}{2m}\right)^2 + \frac{4\pi a\hbar^2 N_0}{mV}\left(\frac{\hbar^2 k^2}{2m}\right)\right]^{1/2} \qquad (3)$$

and the spectral intensivity enables us to find the occupation number of non-condensed excitons:

$$N_{\vec{k}} \equiv \langle B^+_{\vec{k}} B_{\vec{k}} \rangle = \frac{1}{2\mathcal{E}(\vec{k})} \left[\frac{\hbar^2 k^2}{2m} + \frac{2\pi a \hbar^2 N_0}{mV} - \mathcal{E}(\vec{k}) \right]. \qquad (4)$$

The optical properties of the system are determined by the electrical susceptibility tensor χ_{ij} connecting polarization $\vec{P}$ and electric field $\vec{E}$ in the following way: $P_i = 4\pi \chi_{ij} E_j$ .On the other hand, as it was shown in /2/, Chap. IV, the transverse electric susceptibility tensor $\chi^{\perp}_{ij}$ can be expressed over the retarded exciton Green's function (2), so that in the domain of the exciton-photon interaction we obtain:

$$\chi^{\perp}_{ij}(\Omega,\vec{k}) = \frac{-d_i d_j \Delta}{2 v \hbar \Omega} \left[\frac{N_{\vec{k}} + 1}{\Omega - \Delta - \mathcal{E}(\vec{k}) + i\delta} - \frac{N_{\vec{k}}}{\Omega - \Delta + \mathcal{E}(\vec{k}) + i\delta} \right] \qquad (5)$$

Here Δ is the excitation energy of an isolated molecule, d_i and d_j are the components of the dipol transition momentum in the molecule, v is the elementary cell volume and Ω is the photon energy.

The light apsorption coefficient in the crystal is proportional to the imaginar part of the tensor $\chi^{\perp}_{ij}$. From (5) we find:

$$\mathrm{Im}\{ \chi^{\perp}_{ij}(\Omega,\vec{k}) \} = \frac{d_i d_j \Delta}{2 v \hbar \Omega} (N_{\vec{k}} + 1)\, \delta[\Omega - \Delta - \mathcal{E}(\vec{k})] - \frac{d_i d_j \Delta}{2 v \hbar \Omega} N_{\vec{k}}\, \delta[\Omega - \Delta + \mathcal{E}(\vec{k})] \qquad (6)$$

Analysis of the above expression shows that in the presence of the condensate the pozitive apsorption of photons occurs in the system at the frequence: $\Omega_1 = \Delta + \mathcal{E}(\vec{k})$ and, also, that the possibility of the negative apsorption of photons (the stimulated emission) exist at the frequence: $\Omega_2 = \Delta - \mathcal{E}(\vec{k})$.

/1/V.M.Agranovich, B.S.Toshich, Sov.Phys.JETP 26, 1o5 (68).
/2/A.S.Davidov, THEORY OF MOLECULAR EXCITON, Nauka, Moscow 1968 (in Russian).