Simple method for collective excitations in multicomponent mixtures of quantum fluids

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We present a simple analytical method to compute the approximate spectrum of elementary collective excitations for hypothetical arbitrarily many-component "electron-hole" fluids. Numerical results are given for two- and ten-component systems in three dimensions and for a six-component system in two dimensions.

Thirty five years ago Feynman showed[1] that a good approximation to low-lying excited states ψ_E of liquid ^{4}He is given by

$$\psi_E=\sum_{j=1}^{N} e^{i\mathbf{k}\cdot\mathbf{r}_j}\psi_0 , \tag{1}$$

where ψ_0 is the ground-state wave function. This leads to excitation energy

$$\epsilon(k)=\frac{\hbar^2k^2}{2mS(k)} , \tag{2}$$

which is valid in the limit $k\rightarrow 0$. $S(k)$ is the liquid structure function which goes to infinity for large values of k when this formula gives the single-particle excitation energy. m is the mass of liquid particles. This description is easily generalized to arbitrarily many-component mixtures of quantum fluids. Then the many branches of the excitation spectrum are obtained as eigenstates of the matrix

$$\frac{\hbar^2k^2}{2}[M^{-1/2}S^{-1}(k)M^{-1/2}] , \tag{3}$$

where $S(k)$ now means the matrix made of pairwise structure functions $S_{\alpha\beta}(k)$, $\alpha,\beta=1,\ldots,n$, n is the number of the components, and $M=\mathrm{diag}(m_\alpha)$ is the diagonal mass matrix. In the present work we apply this method to multicomponent mixtures of charged quantum fluids, both three- and two-dimensional systems.

Approximate ground-state structure functions are obtained by employing the variational method. As a starting point we use the Euler-Lagrange equations written in the form[2]

$$\frac{-\hbar^2}{2\mu_{\alpha\beta}}\nabla^2[g_{\alpha\beta}(\mathbf{r})^{1/2}] +[v_{\alpha\beta}(\mathbf{r})+w_{\alpha\beta}(\mathbf{r})][g_{\alpha\beta}(\mathbf{r})]^{1/2}=0 , \tag{4}$$

where $g_{\alpha\beta}$ $(\alpha,\beta=1,\ldots,n)$ are the pair correlation functions, $v_{\alpha\beta}$ are pairwise potentials, $\mu_{\alpha\beta}$ are reduced masses, and $w_{\alpha\beta}(r)$ the elements of the matrix whose Fourier transform is

$$w(\mathbf{k})=\frac{-\hbar^2k^2}{4}\{[S(\mathbf{k})MS(\mathbf{k})]^{-1}-[S_F(\mathbf{k})MS_F(\mathbf{k})]^{-1} +M^{-1}[S(\mathbf{k})-1]+[S(\mathbf{k})-1]M^{-1}\} . \tag{5}$$

Here S_F is a diagonal matrix made of noninteracting structure functions. We can rewrite the Euler-Lagrange equation (4) in momentum space as

$$[S(\mathbf{k})MS(\mathbf{k})]^{-1}=[S_F(\mathbf{k})+MS_F(\mathbf{k})]^{-1}+\frac{4}{\hbar^2k^2}v(\mathbf{k}) -\frac{2}{k^2}[M^{-1}R(\mathbf{k})+R(\mathbf{k})M^{-1}] , \tag{6}$$

where $v(\mathbf{k})$ is the matrix of the pair potentials. $R(\mathbf{k})$ is a matrix whose components in r space are defined as

$$R_{\alpha\beta}(\mathbf{r})=\frac{1}{2}\left[\frac{1-g_{\alpha\beta}}{g_{\alpha\beta}}\right]\nabla^2g_{\alpha\beta}-\frac{1}{4}\left[\frac{\nabla g_{\alpha\beta}}{g_{\alpha\beta}}\right]^2 , \tag{7}$$

and we use a dimensionless Fourier transform

$$a(\mathbf{k})=(\rho_\alpha\rho_\beta)^{1/2}\int e^{i\mathbf{k}\cdot\mathbf{r}}a(\mathbf{r})d\mathbf{r} , \tag{8}$$

where ρ_α (ρ_β) is the number density of component α (β). Equation (6) may be a useful starting point in deriving iterative methods for solving the complete set of the Euler-Lagrange equations.

Multiplying Eq. (6) from both sides with $(k^2/2)M^{-1/2}$ we obtain

$$\left[\frac{k^2}{2}(M^{-1/2}S^{-1}M^{-1/2})\right]^2=\left[\frac{k^2}{2}(M^{-1/2}S_F^{-1}M^{-1/2})\right]^2+M^{-1/2}[k^2v(\mathbf{k})]M^{-1/2} -\tfrac{1}{2}k^2M^{-1/2}(M^{-1}R+RM^{-1})M^{-1/2} . \tag{9}$$

From this form we see directly that the collective excitations are the square roots of the eigenvalues of the right-hand side of Eq. (9). In Coulomb systems, which are not too strongly correlated, we obtain a good approximation already by dropping the $R(k)$ term in the right-hand side of Eq. (9). This is useful because then we can handle n components almost as easily as only one.

As an example we consider hypothetical two- and ten-component "electron-hole" systems in two and three dimensions. We first compare the excitation curves and structure functions calculated from Eq. (9) and from the approximate equation

$$[S(\mathbf{k})MS(\mathbf{k})]^{-1}=[S_F MS_F(\mathbf{k})]^{-1}+\frac{4}{\hbar^2 k^2}v(\mathbf{k}) , \tag{10}$$

which we get by dropping the terms depending on $g_{\alpha\beta}$ in Eq. (9). In three dimensions[3]

$$S_F=\begin{cases}\frac{3}{4}(k/k_F)-\frac{1}{16}(k/k_F)^3, & k\le 2k_F\\ 1, & k>2k_F .\end{cases} \tag{11}$$

Figure 1 presents the collective excitation energies for a two-component fluid where the mass ratio of the components $m_2/m_1=3$. The length scale is defined here in terms of the first component mass M_1, i.e., $a_0=\hbar^2/m_1e^2$, and the energy unit is 1 Ry$=\frac{1}{2}e^2/a_0$. The dimensionless density parameter is also defined in terms of the first-component density $r_s=(3/4\pi\rho_1)^{1/3}/a_0$. The dashed and solid curves represent the full and approximate equations (9) and (10), respectively. The dashed-dotted curve represents the result of Vignale and Singwi[4] who applied a method utilizing a generalized random-phase approximation. The fully iterated equations which include the effect of short-range correlations give, not surprisingly, slightly lower energy than the approximate equation (10) and the result of Ref. 4.

In Fig. 2 we show excitation spectra for two different ten-component fluids. Just for curiosity we chose the

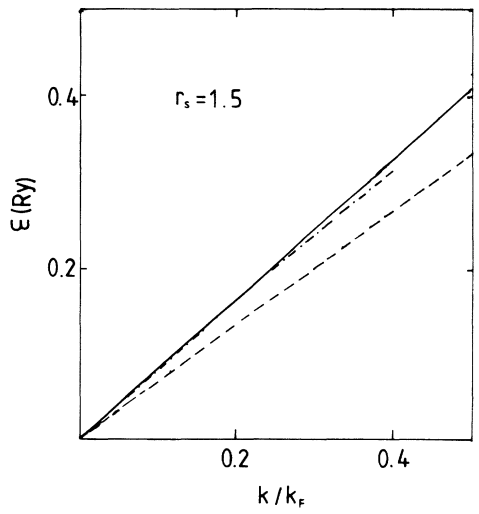

FIG. 1. Collective excitation for a two-component fluid with $m_2/m_1=3$ at $r_s=1.5$. The solid curve presents the approximation of Eq. (10), the dashed curve presents the eigenvalues of Eq. (9), and the dash-dotted curve shows the result of Ref. 4.

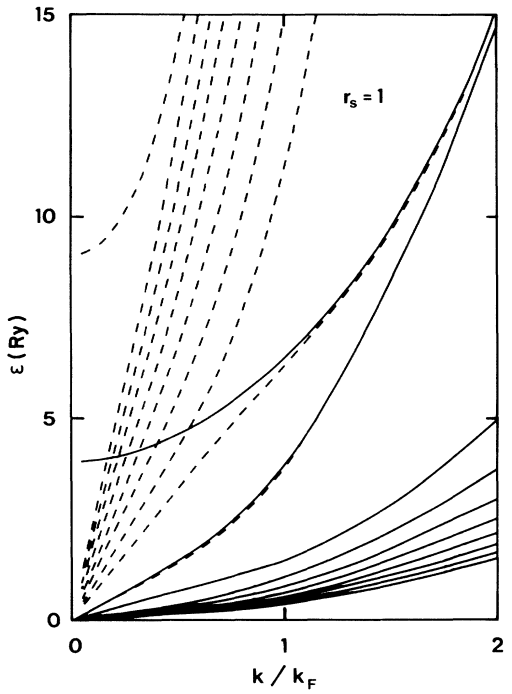

FIG. 2. Excitation spectra for two ten-component fluids. The solid line represents a system which consists of one electron component and nine hole components whose mass ratios are $m_\alpha/m_1=+1,3,\ldots,10$, $\alpha=2,3,\ldots,10$. The dashed lines represent a system where the masses of the nine hole components are $1,\frac{1}{2},\ldots,$ and $\frac{1}{10}$ times the electron mass.

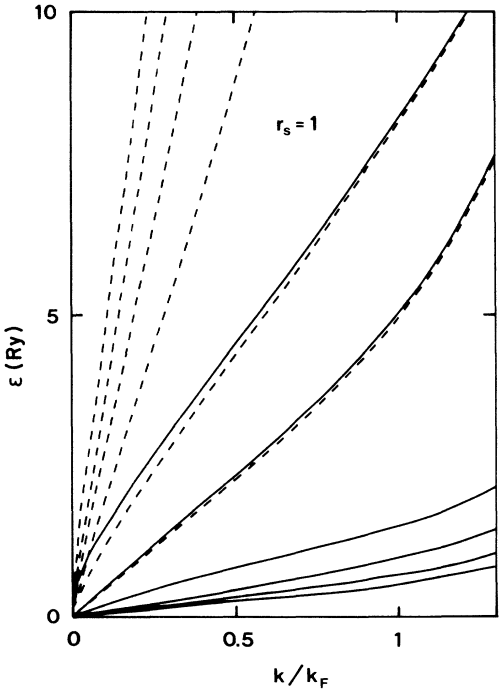

FIG. 3. Excitation spectra for two six-component two-dimensional fluids at $r_s=1$. Two of the components have the same mass, the others having mass ratios $m_\alpha/m_1=4$, 6, 8, and 10 (solid lines) and $\frac{1}{4}$, $\frac{1}{6}$, $\frac{1}{8}$, and $\frac{1}{10}$ (dashed lines).

number of components to be ten: say, one "electron" and nine "hole" components with opposite charge. In the first, heavy-hole system, represented by solid lines, the masses of the hole components are chosen to be heavier than the electron mass: $m_\alpha/m_1=1,3,\ldots,10$ for $\alpha=2,3,\ldots,10$.

In the second, light-hole system, the mass ratios are, respectively, $m_\alpha/m_1=1,\frac{1}{2},\ldots,\frac{1}{10}$. In both cases the overall neutrality is guaranteed by choosing the density of each hole component to be $\rho_\alpha=\rho_1/9$, $\alpha=2,\ldots,10$. In these multicomponent systems there is only one plasma mode, whose frequency at $k=0$ is

$$\omega_p^2=4\pi e^2\sum_{\alpha=1}^{n}\frac{\rho_\alpha}{m_\alpha}\ , \tag{12}$$

and the rest of the modes are phonons, i.e., their energy is linear in k as $k\to 0$.

In the two systems, described in Fig. 2, one hole-component mass equals that of the electron. Hence two branches in both systems merge as $k\to\infty$. In the heavy-hole system the plasmon mode and the highest phonon mode merge. In the light-hole system, because the dispersion curves cannot cross each other, the steeply rising phonon modes push the plasmon mode up, and two lowest phonon modes approach each other asymptotically.

In two dimensions $v(k)=(2/r_s)(2\pi\rho/k)$ and[5]

$$S_F(k)=\begin{cases}\dfrac{2}{\pi}\left\{\arcsin\left[\dfrac{k}{2k_F}\right]+\dfrac{k}{2k_F}\left[1-\left[\dfrac{k}{2k_F}\right]^2\right]^{1/2}\right\}, & k\le 2k_F\\ 1, \quad k>2k_F\ .\end{cases} \tag{13}$$

Taking this into account we find the excitation curves of Fig. 3 for a two-dimensional system. Qualitatively, the main difference between the two- and three-dimensional systems is that in 2D, the plasmon energy does not go to constant as $k\to 0$, but approaches zero as $\sqrt{k}$.

In this work we have considered the collective modes of multicomponent "electron-hole" systems. In fermionic systems these modes, except plasmons, are inside the single-particle continuum and therefore are not realizable as stable excitations. In bosonic systems the situation would be different. However, analogous methods may find interesting applications in handling some problems in superlattice and quantum wire systems, which may be directly mapped to multicomponent systems.

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