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Rotons and the density matrix of liquid ^{4}He

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A density matrix for liquid ^{4}He is constructed starting from the elementary-excitation picture. Rotons are described by the Feynman-Cohen wave function. This generalizes Penrose's form for the density matrix that is based on the Feynman form for the wave function. Backflow introduces explicit temperature-dependent three- and four-body correlations in the density matrix in the coordinate representation. We have computed the effect of the backflow terms, with the omission of the four-body one, on the structure factor $S(k,T)$ on the basis of the random-phase approximation and of the convolution approximation for the triplet structure factor. We find improved agreement with experiment on the temperature dependence of $S(k,T)$.

The ground-state properties of strongly interacting Bose fluids, in particular liquid ^{4}He, are now fairly well understood by working directly with the ground-state wave function: The Jastrow variational method[1] and the Green-function Monte Carlo method[2] represent the basic approaches in the field. At finite temperature many properties of the system can be obtained without working at such a detailed level and only the structure of the excited states are needed. Recall the famous Landau theory of superfluid helium.[3] For other quantities, however, this is not enough and this is the case, for instance, of the momentum distribution and of the radial distribution function needed to compute the structure factor $S(q)$. The full density matrix in the coordinate representation is required in such cases.

Penrose[4] obtained long ago the density matrix for an ideal gas of phonons propagating in a Bose fluid. The wave function of such phonons was assumed to have the Feynman form

$$\Psi^F_{\vec{k}}(\vec{r}_1,\ldots,\vec{r}_N)=\frac{\rho_{\vec{k}}}{[NS_0(k)]^{1/2}}\Psi_0(\vec{r}_1,\ldots,\vec{r}_N)\ , \tag{1}$$

where Ψ_0 is the ground-state wave function and $S_0(k)$ is the related structure factor. $\rho_{\vec{k}}$ is the $\vec{k}$ component of the microscopic density,

$$\rho_{\vec{k}}=\sum_j \exp(i\vec{k}\cdot\vec{r}_j)\ .$$

Penrose's density matrix is appropriate at low temperature where only long-wavelength phonons are thermally excited, say T below 0.5 K in ^{4}He. At higher temperature short-wavelength excitations, the so-called rotons, become important. In order to treat this case Penrose's density matrix has been empirically generalized by Feenberg[5] by extending the sum over the states also to the roton region, still assuming the Feynman form (1) for the excited-state wave function. However, it is well known that the excitation energy given by (1),

$$\epsilon(k)=\hbar^2k^2/2mS_0(k)\ ,$$

is in strong disagreement with experiments in the roton region. In fact $\Psi^F_{\vec{k}}$ neglects any correlation in addition to those present in Ψ_0 whereas it is known that rotons have specific interparticle correlations, the so-called backflow effect. The standard form that takes into account this backflow is the Feynman-Cohen (FC) form,[6]

$$\Psi^{\mathrm{FC}}_{\vec{k}}(\vec{r}_1,\ldots,\vec{r}_N)=\frac{1}{(N\mathcal{N}_k)^{1/2}}\sum_j e^{i\vec{k}\cdot\vec{r}_j}\left[1+i\sum_{\substack{l\\ l\neq j}} g_{\vec{k}}(\vec{r}_j-\vec{r}_l)\right]\Psi_0\ , \tag{2}$$

$$g_{\vec{k}}(\vec{r})=A_k\vec{k}\cdot\vec{r}/r^3\ , \tag{3}$$

where $\mathcal{N}_k$ is the normalization constant and A_k is the constant that minimizes the expectation value of the energy.

In this paper we show that Penrose's density matrix can be generalized by considering an ideal gas of excitations described by a Feynman-Cohen wave function. This density matrix turns out to have explicit temperature-dependent three- and four-body correlations, in addition to the two-body ones present in Penrose's density matrix.

We consider a Bose fluid of N particles at rest. The density matrix in the coordinate representation reads as follows:

$$\langle R'|\sigma|R\rangle=\frac{1}{Z}\sum_{\{n_{\vec{k}}\}}\exp[-\beta E(\{n_{\vec{k}}\})]\Psi^*_{\{n_{\vec{k}}\}}(R')\Psi_{\{n_{\vec{k}}\}}(R)\ , \tag{4}$$

where $R\equiv(\vec{r}_1,\ldots,\vec{r}_N)$, $Z=\sum\exp[-\beta E(\{n_{\vec{k}}\})]$ is the partition function, and $n_{\vec{k}}=0,1,\ldots,$ is the occupation number of the excitation of wave vector $\vec{k}$. Within the picture of independent elementary excitations of spectrum ϵ_k the energy $E(\{n_{\vec{k}}\})$ of a state of multiple excitation is given by

$$E(\{n_{\vec{k}}\})=E_0+\sum_{\vec{k}}n_{\vec{k}}\epsilon_k\ , \tag{5}$$

where E_0 is the ground-state energy, and the wave function reads

$$\Psi_{\{n_{\vec{k}}\}}(R)=[\mathcal{N}(\{n_{\vec{k}}\})]^{-1/2}\times\prod_{\substack{\vec{k}\\ \vec{k}\neq 0}}[F_{\vec{k}}(R)/\sqrt{N}\,]^{n_{\vec{k}}}\Psi_0(R)\;. \tag{6}$$

$\mathcal{N}(\{n_{\vec{k}}\})$ is the normalization constant and $F_{\vec{k}}(R)$ represents the function in large parentheses in (2). It is convenient to rewrite $F_{\vec{k}}(R)$ in terms of the density Fourier components[7]:

$$F_{\vec{k}}(R)=\rho_{\vec{k}}+iA_k\sum_{\vec{q}}\varphi_{\vec{k},\vec{q}}\rho_{\vec{k}-\vec{q}}\rho_{\vec{q}}\;,$$
$$\rho_{\vec{k}}=\sum_j\exp(i\vec{k}\cdot\vec{r}_j)\;. \tag{7}$$

In the FC approximation (3) $\varphi_{\vec{k},\vec{q}}$ is given by

$$\varphi_{\vec{k},\vec{q}}=(4\pi i/V)\vec{k}\cdot\vec{q}/q^2\;. \tag{8}$$

For our purpose A_k must be considered as a known function of k as determined by a separate variational computation of the excitation spectrum. $|A_k|$ has a maximum for k in the roton region and vanishes for $k\to 0$.[6,8]

The construction of the density matrix involves two basic steps. In the first we compute the normalization constant $\mathcal{N}\{n_{\vec{k}}\}$ and in the second we perform the summation over the states in (4). $\mathcal{N}(\{n_{\vec{k}}\})$ can be considered as the average of

$$\prod_{\vec{k}}(|F_{\vec{k}}|^2/N)^{n_{\vec{k}}}$$

with respect to $|\Psi_0|^2$ so we write

$$\mathcal{N}(\{n_{\vec{k}}\})=\left\langle\prod_{\substack{\vec{k}\\ \vec{k}\neq 0}}(|F_{\vec{k}}|^2/N)^{n_{\vec{k}}}\right\rangle_0\;. \tag{9}$$

Since $F_{\vec{k}}$ is a quadratic form in $\rho_{\vec{q}}$, $\mathcal{N}(\{n_{\vec{k}}\})$ can be written as the average of a polynomial of $\rho_{\vec{q}}$. Such averages have an important factorization property.[9] Let us consider an average of the density variables,

$$I_n(\vec{k}_1,\ldots,\vec{k}_n)=\left\langle\prod_{i=1}^{n}\rho_{\vec{k}_i}\right\rangle\;, \tag{10}$$

with $\sum_i\vec{k}_i=0$. The average is taken with respect to an arbitrary normalized weight function $P(\vec{r}_1,\ldots,\vec{r}_N)$ that is assumed to have the following cluster property: The m-particle reduced-distribution function $g^{(m)}(\vec{r}_1,\ldots,\vec{r}_m)$ becomes $g^{(m-1)}(\vec{r}_1,\ldots,\vec{r}_{m-1})$ when $\vec{r}_m$ is far away from the remaining $m-1$ coordinates. Under these conditions, Wu[9] has proved that for a translationally invariant system the contribution to I_n of higher order in N is the sum of all the possible factorizations of the type

$$\prod_{\alpha=1}^{l}I_{m_\alpha}(\vec{k}_{\alpha_1},\ldots,\vec{k}_{\alpha_{m_\alpha}})\;,$$

with the largest value of l. Here $\sum_\alpha m_\alpha=n$ and each I_{m_α} must conserve the momentum

$$\sum_{i=1}^{m_\alpha}\vec{k}_{\alpha_i}=0\;.$$

For instance,

$$\langle\rho_{\vec{k}_1}\rho_{\vec{k}_2}\rho_{\vec{k}_3-\vec{k}_1-\vec{k}_2}\rho_{-\vec{k}_3}\rho_{\vec{k}_4}\rho_{-\vec{k}_4}\rho_{\vec{k}_4}\rho_{-\vec{k}_4}\rangle=2\langle\rho_{\vec{k}_1}\rho_{\vec{k}_2}\rho_{\vec{k}_3-\vec{k}_1-\vec{k}_2}\rho_{-\vec{k}_3}\rangle\langle\rho_{\vec{k}_4}\rho_{-\vec{k}_4}\rangle^2\left[1+O\left[\frac{1}{N}\right]\right]\;.$$

Using this theorem for the average (9) it is simple algebra to obtain, for instance,

$$\langle|F_{\vec{k}}|^2|F_{\vec{h}}|^2\rangle=(1+\delta_{\vec{k},\pm\vec{h}})\langle|F_{\vec{k}}|^2\rangle\langle|F_{\vec{h}}|^2\rangle\times\left[1+O\left[\frac{1}{N}\right]\right]\;. \tag{11}$$

Similar factorizations can be deduced for higher-order averages by the method used by Jackson and Feenberg[10] in the case of the Feynman wave function. In that case in fact, the factorization (11) holds true when $F_{\vec{k}}$ is substituted by $\rho_{\vec{k}}$ so that we can now replace $\rho_{\vec{k}}$ with $F_{\vec{k}}$ in Jackson-Feenberg computation. For instance, by introducing the generating function,

$$\mathcal{G}(\vec{k},x)=\int d\vec{r}_1\cdots d\vec{r}_N\,|\Psi_0(\vec{r}_1,\ldots,\vec{r}_N)|^2\times\exp(-x\,|F_{\vec{k}}|^2/N)\;, \tag{12}$$

the normalization constant,

$$\mathcal{N}_{\vec{k}}\equiv\langle|F_{\vec{k}}|^2N\rangle_0\;, \tag{13}$$

can be written in term of the generalized one,

$$\mathcal{N}_{\vec{k}}(x)=-\frac{d}{dx}\ln\mathcal{G}(\vec{k},x)\;, \tag{14}$$

as $\mathcal{N}_{\vec{k}}=\mathcal{N}_{\vec{k}}(0)$. Taking the derivative of $\mathcal{N}_{\vec{k}}(x)$ with respect to x and using (11), we find

$$\frac{d}{dx}\mathcal{N}_{\vec{k}}(x)=-\mathcal{N}^2_{\vec{k}}(x)\;. \tag{15}$$

This integrates to

$$\mathcal{N}_{\vec{k}}(x)=\mathcal{N}_{\vec{k}}/(1+x\mathcal{N}_{\vec{k}})$$

and from (14) we obtain

$$\mathcal{G}(\vec{k},x)=(1+x\mathcal{N}_{\vec{k}})^{-1}\;.$$

Expanding this relation and (12) in power series of x and equating the coefficients of x^n, one finds that

$$\langle(|F_{\vec{k}}|^2/N)^n\rangle_0=n!\mathcal{N}^n_k\;.$$

This result can be extended to the case of excitations of different wave vectors[10] and we get

$$\mathcal{N}(\{n_{\vec{k}}\})=\langle\prod_{\vec{k}}(|F_{\vec{k}}|^2/N)^{n_{\vec{k}}}\rangle_0 =\prod_{\vec{k}} n_{\vec{k}}!\mathcal{N}_{\vec{k}}^{n_{\vec{k}}} \, . \tag{16}$$

Comparison of this expression with that obtained with the Feynman wave function indicates a formal identity between the two cases, with $\rho_{\vec{k}}/[NS_0(k)]^{1/2}$ being replaced by $F_{\vec{k}}/(N\mathcal{N}_{\vec{k}})^{1/2}$ in the present case. $S_0(k)$ is the ground-state structure factor and the normalization constant $\mathcal{N}_{\vec{k}}$ of a single excitation reads[6]

$$\mathcal{N}_{\vec{k}}=S_0(k)+kA_kI_9(k)+k^2A_k^2I_{10}(k) \, , \tag{17}$$

where I_9 and I_{10} are three- and four-particle integrals entering the FC theory.

This formal identity allows us to perform the sum over the states in (3) with the same technique used by Penrose or by Feenberg, and the density matrix reads

$$\begin{gathered}\langle R'|\sigma|R\rangle=Q_N^{-1}\Psi_0^*(R')\Psi_0(R)\prod_{\substack{\vec{k}\\ k_x>0}}\langle R'|(k,-k)|R\rangle \, ,\\ \langle R'|(k,-k)|R\rangle=[1-\exp(-2\beta\epsilon_k)]\exp\frac{[x'+x'^*-(x+x'')\exp(-\beta\epsilon_k)]\exp(-\beta\epsilon_k)}{1-\exp(-2\beta\epsilon_k)} \, ,\end{gathered} \tag{18}$$

where Q_N is the normalization constant and

$$x=F_{\vec{k}}(R)F_{-\vec{k}}(R)/N\mathcal{N}_{\vec{k}} \, ,$$

$$x'=F_{\vec{k}}(R)F_{-\vec{k}}(R')/N\mathcal{N}_{\vec{k}} \, ,$$

$$x''=F_{\vec{k}}(R')F_{-\vec{k}}(R')/N\mathcal{N}_{\vec{k}} \, .$$

Taking into account the form [Eqs. (7) and (8)] for $F_{\vec{k}}$ one can easily write $\langle R'|\sigma|R\rangle$ in terms of the particle coordinates and one finds two-, three-, and four-body terms. In particular the diagonal term reads

$$\langle R|\sigma|R\rangle=Q_N^{-1}|\Psi_0(R)|^2\exp\left[-\frac{1}{2}\sum_{\substack{i,j\\ i\neq j}}u_T(|\vec{r}_i-\vec{r}_j|)-\sum_{\substack{i,j,l\\ i\neq j\neq l}}u_T^{(3)}(\vec{r}_i,\vec{r}_j,\vec{r}_l)-\sum_{\substack{i,j,l,s\\ i\neq j\neq l\neq s}}u_T^{(4)}(\vec{r}_i,\vec{r}_j,\vec{r}_l,\vec{r}_s)\right] \, , \tag{19}$$

where the temperature-dependent correlation terms can be written in the form

$$u_T(r)=h_0(r)+\frac{2}{r^2}h_1'(r)+\frac{1}{r^4}h_2''(r) \, , \tag{20}$$

$$u_T^{(3)}(\vec{r}_1,\vec{r}_2,\vec{r}_3)=h_1'(r_{12})\frac{\vec{r}_{12}\cdot\vec{r}_{13}}{r_{12}r_{13}^3}+2h_2''(r_{12})\frac{\vec{r}_{12}\cdot\vec{r}_{13}}{r_{12}^3r_{13}^3} \, , \tag{21}$$

$$u_T^{(4)}(\vec{r}_1,\vec{r}_2,\vec{r}_3,\vec{r}_4)=h_2''(r_{12})\frac{\vec{r}_{12}\cdot\vec{r}_{13}}{r_{12}r_{13}^3}\frac{\vec{r}_{21}\cdot\vec{r}_{24}}{r_{21}r_{24}^3} \, , \tag{22}$$

where h_α' and h_α'' denote, respectively, the first and the second spatial derivative of h_α and we have introduced the auxiliary functions,

$$h_\alpha(r)=\frac{1}{N}\sum_{\vec{k}}\frac{A_k^\alpha}{\mathcal{N}_k}\frac{-2\gamma_k}{\gamma_k+1}\exp(i\vec{k}\cdot\vec{r}) \quad (\alpha=0,1,2) \tag{23}$$

$$\gamma_k=\exp(-\beta\epsilon_k) \, , \tag{24}$$

that relates the correlations to the parameters A_k and $\mathcal{N}_k$ of the Feynman-Cohen wave function. ϵ_k is the energy computed with the FC theory.

This completes the formal derivation of the density matrix. From the development of the FC theory it results that the main contribution of the backflow is due to terms linear in A_k, so that it is reasonable to neglect $h_2(r)$. In this case only two- and three-body terms enter $\langle R|\sigma|R\rangle$. The energy spectrum ϵ_k in the Boltzmann factor (24) should be the one computed with the FC theory, but one could also use the empirical spectrum. The elementary excitation picture we have assumed does not take into account the interaction between the excitations that leads to a temperature-dependent spectrum $\epsilon_k(T)$. A mean-field argument[5] suggests that the effect of such interactions can be roughly taken into account by using in (24) this empirical spectrum $\epsilon_k(T)$.

We conclude that the Penrose density matrix can be generalized by taking into account backflow terms in the wave function of a single excitation. If a form of the wave function different from the FC one were to be used for the excited states this would not alter the basic structure of σ but only the expression [Eqs. (20)–(22)] of the correlation terms. This new density matrix differs from the Penrose form mainly for the correlations at intermediate distances since A_k is large only for k in the roton region. For this reason the computation of the temperature dependence of the structure factor $S(k,T)$ appears very interesting. On the basis of the Penrose density matrix the anomalous T dependence of $S(k,T)$ has been interpreted[11] as an effect of the thermal population of roton states. This should be confirmed by a computation based on the new density matrix that starts from a much better wave function for rotons.

The main result of the computation[11] of Gaglione *et al.* is that this thermal effect makes the main peak of $S(k,T)$ higher and sharper as the temperature increases, at least as long as rotons remain well-defined elementary excitations of the system. Good agreement with experiment has been obtained[11] on the amplitude of the effect and on the sharpening of the peak. The only significant discrepancy lies is a small shift in the position of the effect: Experiments show that the position of the main maximum of $S(k,T)$ does not change with T whereas the computation gives a small shift with T due to the fact that the difference $S(k,T)-S_0(k)$ is maximum at $k \approx 1.94$ Å^{-1}, the wave vector of the roton minimum, and not at $k \approx 2.04$ Å^{-1}, the position of the main peak of $S_0(k)$. Since the density matrix we have deduced is based on a better approximation of the roton states, one should verify if this discrepancy is lifted by our density matrix without affecting, at the same time, the points of agreement already present. This computation is very difficult, however, because the problem of computing the structure factor in the presence of three- and four-body correlations is still a practically unsolved statistical-mechanical problem. The use of a simulation method like Monte Carlo with three-body correlations of the form (21) is possible[12] but it is still a major numerical undertaking. Some approximate schemes have been proposed but, unfortunately, there is no comparison with simulation results that benchmarks the approximations. One approximation[13] is based on the replacement of the three-body term by an effective two-body one but this is specific for a low-density system. Another approach[14] is based on the random-phase approximation (RPA) and the convolution approximation for the triplet structure factor. At the level of two-body correlations it is known[11] that the RPA is very poor; it overestimates $S(k,T)-S_0(k)$ by a factor of 3 and it does not give any sharpening of the peak. However, it gives correctly the position of the maximum of $S(k,T)-S_0(k)$. On this basis we do not expect that RPA will give reliable results for the effect of the three-body term. However, this approximation might be appropriate to answer the question if the backflow term lifts the discrepancy between experiment and the Penrose density matrix result concerning the position of the maximum of $S(k,T)$.

Application of the theory of Ref. 14 to the density matrix (19) is straightforward if we neglect $u_T^{(4)}$ and if we assume that ψ_0 is of the Jastrow form,

$$\prod_{\substack{i,j\\ i<j}} f(r_i-r_j) \, .$$

The structure factor reads

$$S(k,T)=S_2(k,T)\exp\left[\frac{S_2(k,T)}{2}F(k,T)\right] , \tag{25}$$

$$F(k,T)=\frac{1}{(2\pi)^3}\int d^3q[S_2(|\vec{k}+\vec{q}|,T)S_2(q,T)-1]4\pi\frac{\vec{q}\cdot(\vec{q}+\vec{k})}{|\vec{q}+\vec{k}|^2}\nu_{q'} , \tag{26}$$

$$\nu_k=-\frac{2\gamma_k}{1+\gamma_k}\frac{A_k}{\mathcal{N}_k} , \tag{27}$$

where γ_k and $\mathcal{N}_k$ are given by (24) and (17). $S_2(k,T)$ is the structure factor due to only two-body correlations, i.e., (19) with $u_T^{(3)}=u_T^{(4)}=0$. For consistency we compute the effect of the temperature-dependent two-body term $u_T(r)$ in RPA so that[11]

$$S_2(k,T)=S_0(k)/[1+\rho S_0(k)u_T(k)] , \tag{28}$$

where $u_T(k)$ is the Fourier transform of $u_T(r)$, Eq. (20), that can be written in the form

$$u_T(k)=-\rho^{-1}\mathcal{N}_k^{-1}\frac{2\gamma_k}{1+\gamma_k}-S_0(k)Y(k) , \tag{29}$$

$$Y(k)=\pi^{-2}\int d^3q\frac{\vec{q}\cdot(\vec{q}+\vec{k})}{|\vec{q}+\vec{k}|^2}\nu_q . \tag{30}$$

We have computed numerically the integrals (26) and (30) using for $S_0(k)$ the experimental data[15] at 1 K, the roton parabola[16]

$$\epsilon_k=\Delta+\hbar^2(k-k_0)^2/2\mu$$

with $\Delta=8.67$ K, $k_0=1.936$ Å, and $\mu=0.15m_{\text{He}}$ for the excitation spectrum and Padmore and Chester's results[8] for the backflow parameters A_k, $I_9(k)$, and $I_{10}(k)$. We find that the backflow does not modify greatly $S(k,T)-S_0(k)$; it enhances the value of the maximum and displaces slightly its position, in better agreement with experiment. For instance at $T=1.8$ K the maximum of $S(k,T)-S_0(k)$ is found at $k=2.0$ Å^{-1} against the value $k=1.94$ Å^{-1} when $A_k=0$. We have already mentioned that RPA is completely inadequate to give the shape and amplitude of $S(k,T)-S_0(k)$ so that we do not report such results.

We conclude that within RPA the presence of the backflow term more than halves the difference in the position of the maximum of $S(k,T)-S_0(k)$ between experiment and theory without backflow. It is gratifying to find such an improvement but, as we already noticed, RPA for three-body correlations has not really been tested yet and we must await a computation based on simulation methods in order to assess if the new density matrix fully explains the observed temperature dependence of $S(k,T)$ of superfluid ^{4}He.

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