Density collective oscillations and single-particle excitations in an ensemble of interacting identical particles

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Abstract

It is shown that apart from the non-integrable (chaotic) "Zitterbewegung" of individual particles, an ensemble of interacting particles exhibits collective oscillations of the particle density (collective excitations) with small amplitudes in the long wavelength limit. The single-particle excitations (quasiparticles) of the ensemble are also defined. All these (collective and single-particle) excitations correspond to an emergent dynamics, requiring additional assumptions about the underlying motion.

We consider N identical particles with mass m in volume V interacting through the pair-wise potential $\varphi(|\mathbf{r}_i - \mathbf{r}_j|)$, where i, j label the particles. In order to study the density oscillations we define first a (unique) equilibrium, ground-state. The density oscillations are defined as small deviations with respect to this ground state. Consequently, we assume that there exist equilibrium positions $\mathbf{r}_i^0$, such that the particle density

$$n_0(\mathbf{r}) = \sum_i \delta(\mathbf{r}_i - \mathbf{r}_i^0) = \frac{1}{V} \sum_{\mathbf{q}} e^{i\mathbf{q}\mathbf{r}} \sum_i e^{-i\mathbf{q}\mathbf{r}_i^0} \tag{1}$$

is constant $n_0(\mathbf{r}) = n$. This may happen if and only if the $\mathbf{r}_i^0$ are continuously distributed, such that

$$n_0(\mathbf{r}) = \frac{1}{V} \sum_{\mathbf{q}} e^{i\mathbf{q}\mathbf{r}} \int \frac{d\mathbf{r}'}{a^3} e^{-i\mathbf{q}\mathbf{r}'} = \frac{1}{a^3} = n \ , \tag{2}$$

where a is the mean inter-particle spacing. This is equivalent with the random phase approximation (RPA) and with neglecting the "Zitterbewegung" of the particles. It is noteworthy that the continuous distribution of the sites $\mathbf{r}_i^0$ ensures the uniqueness of the ground-state.[1] For electric charges moving against a neutralizing, continuous, rigid background these assumptions are known to define the "jellium" model. The motion is described by (small) coordinates $\mathbf{u}(\mathbf{r}_i^0)$ defined by

$$\mathbf{r_i} = \mathbf{r}_i^0 + \mathbf{u}(\mathbf{r}_i^0) \ . \tag{3}$$

The kinetic energy is given by

$$T = \frac{1}{2} \sum_i m\dot{\mathbf{r}}_i^2 = \frac{1}{2} \sum_i m\dot{\mathbf{u}}_i^2 = \frac{1}{2}mn \int d\mathbf{r}\dot{\mathbf{u}}^2(\mathbf{r}) = \frac{1}{2}m \sum_{\mathbf{q}} \dot{\mathbf{u}}(\mathbf{q})\dot{\mathbf{u}}(-\mathbf{q}) \ , \tag{4}$$

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[1] A similar view has been expressed by R. Zwanzig, Phys. Rev. **A156** 190 ((1967).

where the Fourier transform

$$\mathbf{u}(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{q}} \mathbf{u}(\mathbf{q}) e^{i\mathbf{q}\mathbf{r}} \ , \ \mathbf{u}(\mathbf{q}) = \frac{\sqrt{N}}{V} \int d\mathbf{r}\mathbf{u}(\mathbf{r}) e^{-i\mathbf{q}\mathbf{r}} \tag{5}$$

is used.

During the motion, the density of particles given by equation (1) suffers a small change given by

$$\delta n(\mathbf{r}) = -\frac{i}{V} \sum_{\mathbf{q}} e^{i\mathbf{q}\mathbf{r}} \sum_{i} \mathbf{q}\mathbf{u}(\mathbf{r}_i^0) e^{-i\mathbf{q}\mathbf{r}_i^0} = -\frac{in}{V} \sum_{\mathbf{q}} e^{i\mathbf{q}\mathbf{r}} \int d\mathbf{r}'\mathbf{q}\mathbf{u}(\mathbf{r}') e^{-i\mathbf{q}\mathbf{r}'} = -ndiv\mathbf{u}(\mathbf{r}) \tag{6}$$

(such that the number of particles is conserved), providing $\mathbf{q}\mathbf{u}(\mathbf{r}_i^0) \ll 1$. Its Fourier transform reads

$$\delta n(\mathbf{q}) = -in\mathbf{q}\mathbf{u}(\mathbf{q}) \ . \tag{7}$$

Similarly, the interaction is given by

$$U = \frac{1}{2} \sum_{i \neq j} \varphi(|\mathbf{r}_i - \mathbf{r}_j|) = \frac{1}{2} \int d\mathbf{r}d\mathbf{r}'\varphi(|\mathbf{r} - \mathbf{r}'|)\delta n(\mathbf{r})\delta n(\mathbf{r}') \ , \tag{8}$$

or

$$U = \frac{1}{2n} \sum_{\mathbf{q}} \varphi(q)\delta n(\mathbf{q})\delta n(-\mathbf{q}) \ , \tag{9}$$

where $\varphi(q)$ is the Fourier transform of the interaction potential,

$$\varphi(r) = \frac{1}{V} \sum_{\mathbf{q}} \varphi(q) e^{i\mathbf{q}\mathbf{r}} \ . \tag{10}$$

We can see from equations (7) and (9) that the interaction implies only longitudinal coordinates $\mathbf{u}(\mathbf{q})$ along the wavevector $\mathbf{q}$, so we may write $\mathbf{u}(\mathbf{q}) = (\mathbf{q}/q)u(\mathbf{q})$, $\delta n(\mathbf{q}) = -inqu(\mathbf{q})$, with $\delta n^*(-\mathbf{q}) = \delta n(\mathbf{q})$, $\mathbf{u}^*(-\mathbf{q}) = \mathbf{u}(\mathbf{q})$ and $u^*(-\mathbf{q}) = -u(\mathbf{q})$. Making use of these coordinates the kinetic energy given by equation (4) becomes

$$T = -\frac{1}{2}m \sum_{\mathbf{q}} \dot{u}(\mathbf{q})\dot{u}(-\mathbf{q}) \tag{11}$$

and the potential energy given by equation (9) reads

$$U = -\frac{1}{2}n \sum_{\mathbf{q}} q^2\varphi(q)u(\mathbf{q})u(-\mathbf{q}) \ . \tag{12}$$

The classical equations of motion corresponding to the lagrangian $L = T - U$ are[2]

$$m\ddot{u}(\mathbf{q}) + nq^2\varphi(q)u(\mathbf{q}) = 0 \ . \tag{13}$$

They describe density collective oscillations with frequency given by $\omega^2 = nq^2\varphi(q)/m$. As it is well-know, these oscillations are sound waves for short-range potentials and plasma waves for the Coulomb potential ($\varphi(q) = 4\pi ne^2/m$, where e is the particle charge). They can be quantized as usually. They do contribute to the thermodynamics of the ensemble, in the usual way. They

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[2]It is worth noting that the dynamics of these collective coordinates does not depend on the equilibrium sites $\mathbf{r}_i^0$, as expected. It is an emerging dynamics.

have also a finite lifetime, arising both from their mutual interaction (moderate value of $\mathbf{qu}(\mathbf{r}_i^0)$) and from their interaction with the motion of the individual particles (the corresponding coupling arises from the kinetic interaction[3]

The existence of the ground-state defined by continuously-distributed fixed positions $\mathbf{r}_i^0$ is a valid assumption as long as we neglect the movements of individual particles. We give up this assumption here for the moment, and analyze the motion including the "Zitterbewegung" of the particles. The coordinates are now $\mathbf{r}_i$ and the ground-state is the vacuum. The kinetic energy given by equation (4) is

$$T = \frac{1}{2} \sum_i m \dot{\mathbf{r}}_i^2 \tag{14}$$

and the potential energy given by equation (8) reads now

$$U = \frac{1}{2} \sum_{i \neq j} \varphi(|\mathbf{r}_i - \mathbf{r}_j|) = \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \varphi(|\mathbf{r} - \mathbf{r}'|) n(\mathbf{r}) n(\mathbf{r}') \ , \tag{15}$$

where

$$n(\mathbf{r}) = \sum_i \delta(\mathbf{r} - \mathbf{r}_i) = \frac{1}{V} \sum_{\mathbf{q}} e^{i\mathbf{q}\mathbf{r}} \sum_i e^{-i\mathbf{q}\mathbf{r}_i} \ . \tag{16}$$

Making use of equation (16), the potential energy given by equation (15) becomes

$$U = \frac{1}{2V} \sum_{\mathbf{q}} \varphi(q) \sum_{i \neq j} e^{i\mathbf{q}(\mathbf{r}_i - \mathbf{r}_j)} \ . \tag{17}$$

The classical equations of motion are

$$m\ddot{\mathbf{r}}_i - \frac{1}{V} \sum_{\mathbf{q}} \varphi(q) \sum_j \mathbf{q} \sin \mathbf{q}(\mathbf{r}_i - \mathbf{r}_j) = 0 \ , \tag{18}$$

where condition $j \neq i$ is superfluos.

Equations (18) are non-integrable. Indeed, if we multiply both sides of equation (18) with $\dot{\mathbf{r}}_i$ we get

$$\frac{dE_i}{dt} = \frac{1}{V} \sum_{\mathbf{q}} \varphi(q) \sum_j \mathbf{q}\dot{\mathbf{r}}_j \sin \mathbf{q}(\mathbf{r}_i - \mathbf{r}_j) \ , \tag{19}$$

or

$$dE_i = \frac{1}{V} \sum_{\mathbf{q}} \varphi(q) \sum_j \mathbf{q}d\mathbf{r}_j \sin \mathbf{q}(\mathbf{r}_i - \mathbf{r}_j) \ , \tag{20}$$

where

$$E_i = \frac{1}{2}m\dot{\mathbf{r}}_i^2 + \frac{1}{V} \sum_{\mathbf{q}} \varphi(q) \sum_j \cos \mathbf{q}(\mathbf{r}_i - \mathbf{r}_j) \ . \tag{21}$$

From equation (20) we can see that $\partial E_i / \partial \mathbf{r}_j \neq 0$ for $j \neq i$, while $\partial E_i / \partial \mathbf{r}_i = 0$. It follows that the mixed derivatives $\partial^2 E_i / \partial \mathbf{r}_j \partial \mathbf{r}_i$ do not exist (are both vanishing and non-vanishing). This holds in general for ensembles of interacting particles.[4]

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[3]M. Apostol, J. Theor. Phys. **169** (2008).
[4]See, for instance, M. Apostol, J. Theor.Phys. **152** (2007).

However, a consistent dynamics may emerge from equations (18). Indeed, let us write $\mathbf{r}_i = \mathbf{r}_i^0 + \mathbf{u}_i$ as before. Equations (18) become

$$m\ddot{\mathbf{u}}_i = \frac{1}{V} \sum_{\mathbf{q}} \varphi(q) \sum_j \mathbf{q} \sin \mathbf{q}(\mathbf{r}_i^0 - \mathbf{r}_j^0 + \mathbf{u}_i - \mathbf{u}_j) \ . \tag{22}$$

Then we notice that $\mathbf{u}_i - \mathbf{u}_j$ must be along the wavevector $\mathbf{q}$, so it remains only such a vector in summation (18). For small variations we may take $u_i - u_j = -a\partial u/\partial a$ along this $\mathbf{q}$-vector, and also $u_i = a\partial u/\partial a$. Thereafter, we use $\sum_j \cos \mathbf{q}(\mathbf{r}_i^0 - \mathbf{r}_j^0) = N\delta_{\mathbf{q},0}$ and $\sum_j \sin \mathbf{q}(\mathbf{r}_i^0 - \mathbf{r}_j^0) = 0$, and get finally

$$m\partial\ddot{u}/\partial a = -n\varphi(q)q^2\partial u/\partial a \ , \tag{23}$$

which leads to a frequency given by $\omega^2 = nq^2\varphi(q)/m$ in the limit of vanishing q. This way, we recover the density collective oscillations derived above.

Moreover, the RPA applied directly to equation (18) leads to $\mathbf{r}_i = \mathbf{r}_i(\mathbf{q})$ directed along the $\mathbf{q}$-wavevector and oscillating with the collective oscillations frequency given by $\omega^2 = nq^2\varphi(q)/m$ in the long wavelength limit $q \to 0$ (where, however, these oscillations do not exist, as they are absorbed by the motion of the individual particles; the equilibrium, thermodynamic sound exists there, as another elementary collective excitation; it has a finite lifetime, and its contribution to thermodynamics is rather a higher-order effect. Generally, the collective excitations bring a small contribution to the thermodynamics; the main one is brought by the single-particle excitations).

The quantum motion brings nothing new. Indeed, the particle momentum is $\dot{\mathbf{p}}_i = m\dot{\mathbf{r}}_i$, and, making use of the commutator

$$[\mathbf{p}_i, i\mathbf{q}(\mathbf{r}_j - \mathbf{r}_k)] = \hbar\mathbf{q} \left(\delta_{ij} - \delta_{ik} \right) \ , \tag{24}$$

we get

$$\left[\mathbf{p}_i, e^{i\mathbf{q}(\mathbf{r}_j-\mathbf{r}_k)}\right] = \hbar\mathbf{q} \left(\delta_{ij} - \delta_{ik} \right) e^{i\mathbf{q}(\mathbf{r}_j-\mathbf{r}_k)} \ , \tag{25}$$

and

$$\dot{\mathbf{p}}_i = \frac{i}{\hbar} \left[H, \mathbf{p}_i\right] = \frac{1}{V} \sum_{\mathbf{q}} \varphi(q) \sum_j \mathbf{q} \sin \mathbf{q}(\mathbf{r}_i - \mathbf{r}_j) \ , \tag{26}$$

which is the equation of motion (18). It can also be written as

$$\ddot{\mathbf{p}}_i = \frac{1}{V} \sum_{\mathbf{q}} \varphi(q) \sum_j \mathbf{q}(\mathbf{q}\mathbf{p}_i/m) \cos \mathbf{q}(\mathbf{r}_i - \mathbf{r}_j) \ , \tag{27}$$

where one can see more easily the collective oscillations for long wavelengths and small amplitudes.

The non-integrability and the chaotical character of the underlying "Zitterbewegung" call for a statistical motion (where the continuous distribution of the equilibrium positions is ensured). The emerging excitations, either single-particle or collective, have an essential limitation imbued in their finite lifetime, arising mainly from their interaction with the "Zitterbewegung". It is the mark of non-integrability. It is worth noting that the single-particle excitations are individual particles moving in a mean field (quasiparticles). They contribute mostly to the thermodynamics and cohesion. The inherent non-integrability effects may be cast in multi-particle forces. The latter do contribute to the mean field of pair-wise aggregates excitations.[5]

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[5]See M. Apostol, J. Theor. Phys. **152** (2006).

We turn back now to equations (19)-(21). These tell us that the ensemble may be viewed as consisting of one-particle excitations of energy E_i and an uncertainty in energy given by the *rhs* of equation (19). Equation (21) can be written with a satisfactory approximation as

$$E_i = \frac{1}{2} m \dot{\mathbf{r}}_i^2 + n\varphi(0) \qquad (28)$$

This is the energy of a single-particle excitation. It may also define an effective mass (which depends on velocity). It shows that the effect of interaction is a mean field given by the second term in the *rhs* of equation (28). It is very interesting to note the effect of this mean field

$$h = n\varphi(0) = \frac{1}{a^3} \int d\mathbf{r}\,\varphi(\mathbf{r}) \ . \qquad (29)$$

For repulsive short-range potentials $h > 0$, and we have a gas of free particles moving in an external field. Actually, the interaction potential $\varphi(\mathbf{r})$ is repulsive at short distances and attractive at long distances. In such a mean field, the particles may even be trapped, and then we have a cohesion energy $-\varepsilon_0$ per particle and small, local oscillations of the density; together with the kinematical constraint on their motion, the particles form then a liquid.[6] On the other hand, for unbound states we may write

$$h = -\varepsilon_0 = n\varphi(0) \ , \qquad (30)$$

where $-\varepsilon_0$ acts as a cohesion energy. The thermodynamics of such an interacting gas of particles has a free energy

$$F = -NT \ln \left[\frac{eV}{N} (mT/2\pi\hbar^2)^{3/2} \right] - N\varepsilon_0 \ , \qquad (31)$$

and a pressure

$$p = NT/V + N\frac{\partial}{\partial V}\varepsilon_0 \ . \qquad (32)$$

It is easy to find out $N(\partial\varepsilon_0/\partial V) = n^2\varphi(0)$, hence

$$\left[p - n^2\varphi(0) \right] V = NT \ . \qquad (33)$$

Taking into account that $\varphi(0) < 0$, and allowing for an excluded volume, this is van der Waals equation. The equation is valid also for liquids (the difference arises for thermally excited states, which are inhibited in liquids; the energy contains then NT for liquids and $3NT/2$ for monoatomic gases)[7].

Since $m\langle v^2 \rangle /2 = 3T/2$ we get from equation (28) an effective mass change[8]

$$\Delta m/m = \frac{2}{3} n\varphi(0) \ . \qquad (34)$$

The above picture is valid as long as the uncertainty in energy of the single-particle excitations is neglected. We estimate now the *rhs* of equation (19). First, we note that the single-particle excitations with energy E_i given by equation (28) move as free particles, with constant velocities $\mathbf{v}_i$, starting, say, at $\mathbf{r}_i^0$ for $t = 0$. Equation (19) can now be integrated, to give an additional energy

$$\delta E_i = -\frac{1}{V}\sum_{\mathbf{q}}\varphi(q)\sum_j \mathbf{q}\mathbf{v}_j \frac{\cos\left[\mathbf{q}\left(\mathbf{r}_i^0 - \mathbf{r}_j^0\right) + \mathbf{q}(\mathbf{v}_i - \mathbf{v}_j)t\right] - \cos\mathbf{q}\left(\mathbf{r}_i^0 - \mathbf{r}_j^0\right)}{\mathbf{q}(\mathbf{v}_i - \mathbf{v}_j)} =$$

$$= \frac{1}{V}\sum_{\mathbf{q}}\varphi(q)\sum_j \left\{ \cos\left[\mathbf{q}\left(\mathbf{r}_i^0 - \mathbf{r}_j^0\right) + \mathbf{q}\left(\mathbf{v}_i - \mathbf{v}_j\right)t\right] - \cos\mathbf{q}\left(\mathbf{r}_i^0 - \mathbf{r}_j^0\right) \right\} - \qquad (35)$$

$$-\frac{1}{V}\sum_{\mathbf{q}}\varphi(q)\sum_j \mathbf{q}\mathbf{v}_i \frac{\cos\left[\mathbf{q}\left(\mathbf{r}_i^0 - \mathbf{r}_j^0\right) + \mathbf{q}(\mathbf{v}_i - \mathbf{v}_j)t\right] - \cos\mathbf{q}\left(\mathbf{r}_i^0 - \mathbf{r}_j^0\right)}{\mathbf{q}(\mathbf{v}_i - \mathbf{v}_j)} \ .$$

[6]M. Apostol, J.Theor. Phys. **125** (2006).

[7]M. Apostol. J. Theor. Phys. **125** (2006).

[8]M. Apostol and L. C. Cune, J. Theor. Phys. **127** (2006).

The second term in the *rhs* of equation (35) can be neglected in comparison with the first, due to the rapid increase of the denominator, while the summation of the cosines in the first term gives a contribution of the order of unity. It follows

$$\delta E_i \simeq \frac{1}{V} \sum_{\mathbf{q}} \varphi(q) = \varphi(\mathbf{r} = 0) = \varphi_0 \ . \qquad (36)$$

This is a rather high amount of energy. It tells how effective is the interaction in exchanging energy beteeen particles. It may be conceived that such interaction processes ensure a statistical equilibrium, defined by a statistical distribution, with a characteristic energy scale $\varepsilon_{eq} = \varphi_0$. It should be larger than any other relevant energy scale.

It is conceivable that the whole ensemble of particles has a microcanonical distribution $\delta(E - E_0)dE$, as the motion of a closed ensemble conserves the energy. This is unsatisfactory for at least two reasons. First, E is strictly confined to E_0, so the distribution is meaningless. Second, not all the points on the manifold $E(\mathbf{r}_i, \mathbf{p}_i) = E_0$ are reached (ergodic hypothesis, where $\mathbf{p}_i$ is the momentum of the i-th particle), which again makes such a distribution meaningless. We may imagine a solution to these difficulties by assuming a microcanonical distribution for each particle (or sub-ensemble) of the form $\delta(E - E_i - \delta E_i^n)dEdn$, where δE_i^n is the uncertainty in the energy E_i distributed uniformly over over various states n. We may then calculate the mean energy $\overline{E_i} = E_i + \langle \delta E_i \rangle = E_i$ and the mean square deviation from $\overline{E_i^2} = E_i^2 + \langle \delta E_i^2 \rangle$. The difficulty with such a single-particle microcanonical distribution is that it describes each time another particle, as resulting from the collisions processes.

The obvious solution to such difficulties is to ask for the probability for a particle to have a ceratin energy E while the large rest of the ensemble acquires various states. As it is well-known, this probability is given by the canonical distribution

$$\int dE' e^{S'} \delta(E' + E - E_0) = const \times e^{-\beta E} \ , \qquad (37)$$

where $\beta = \partial S'/\partial E'$ for $E' = E_0$ is the inverse of the temperature T and S' is the entropy of the thermal bath. In such terms, the question of the uncertainty δE_i does not appear anymore. Obviously, $\varepsilon_{eq} > T = \varepsilon_{th}$. But the effects of interaction must still be present. We may consider the single-particle excitations with energy as the one given by equation (28), occurring with Gibbs probability given by equation (37) and having a finite lifetime given by interaction. For instance, the particle collisions has cross-section σ, so the quasiparticles has a meanfree path $\Lambda = a^3/\sigma$ and a lifetime $\tau = \Lambda/v$, where v is ofthe order of the thermal velocity ($v \sim \sqrt{T/m}$ for instance). In general, the number of collisions per unit time must be estimated, as governed by interaction, in order to get the lifetime and the meanfree path. The thermodynamics as the one given by equation (31) for such quasiparticles holds. Obviously, the series of inequalities $\varepsilon_{eq} > T > \delta\varepsilon_f > \delta\varepsilon_{ex} (> \delta\varepsilon_q > \delta\varepsilon_{obs})$ is satisfied, where $\delta\varepsilon_f$ is the fluctuation energy per particle, $\delta\varepsilon_{ex}$ is the uncertainty in the quasi-particle (elementary excitation) energy ($\hbar/\tau$), $\delta\varepsilon_q$ is the separation between quantal levels and $\delta\varepsilon_{obs}$ is the uncertainty in energy brought about by the observation. We can see that the single-particle excitations in this picture (statistical or thermodynamical picture) represent an emerging dynamics with respect to the original non-integrable and non-ergodic mechanical ensemble.