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Collective particle hole excitation in a deformed ground state

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It is shown that stable collective particle hole excitations are possible in a generalized Hartree-Fock basis which describes a ground state that has less symmetry than the Hamiltonian. It appears that these collective states remain stable also for strong attractive interaction.

[NUCLEAR STRUCTURE Nuclear matter density fluctuations, generalized random phase approximation.]

It is well known that the Hartree-Fock ground state of an infinite system cannot support collective particle hole excitations for an attractive residual interaction.[1] On the other hand, the breakdown of the random phase approximation (RPA) for attractive interactions is believed to signal the onset of a phase transition which is associated with a broken symmetry of the ground state.[2,3] In the case of an infinite system, the question naturally arises as to whether a nonuniform ground state which breaks translational symmetry exists, and whether this new ground state can support collective quasiparticle quasihole excitations in terms of a suitably chosen single particle basis.

The first question has been answered in the affirmative in a recent paper.[4] It has been shown there that a self-consistent nonuniform density distribution does give rise to a lower total energy of the ground state. The appropriate quasiparticle operators are

$$\Psi^{\dagger}_{\bar{k},m}=\sum_{r=-\infty}^{\infty}\alpha_r^{(m)}(\bar{k})c^{\dagger}_{\bar{k}+rQ} , \tag{1}$$

where the $c_k^{\dagger}$ are plane wave operators and the $\alpha_r^{(n)}(\bar{k})$ are solutions of the self-consistent equations. The fixed momentum value Q determines the "lattice spacing" $d=2\pi/Q$. The total ground state energy is minimized for the value $Q=2k_F$ where the Fermi momentum k_F is determined by the density of the system. The Brillouin zones are characterized by $|\bar{k}|\leq Q/2$. The single particle spectrum $\omega_n(\bar{k})$ shows the same pattern as the one obtained in the band model produced by an external periodic potential.

In this note, we investigate the possibility and the properties of collective density oscillations in this nonuniform medium.

We recall that long wavelength oscillations in a uniform medium with attractive interactions are prevented by the presence of the unperturbed particle hole spectrum which extends from zero to $2k_Fq$ for small momentum transfer q; as a consequence, any collective state with an energy falling into that range would be strongly damped. However, this situation is changed dramatically in the nonuniform medium. Since the first Brillouin zone is just filled in the modified ground state, any unperturbed quasiparticle excitation has to bridge the finite gap between the first and the second energy bands, thus allowing for an undamped collective mode in principle between the two bands. In the following we see that this is in fact possible.

The single particle Green's function for the quasiparticle defined by Eq. (1) is given by

$$G_{\bar{k},m}(\omega)=\frac{n^0}{\omega-\omega_m(\bar{k})-i0}+\frac{1-n^0}{\omega-\omega_m(\bar{k})+i0} , \tag{2}$$

where the occupation number n^0 is unity for $m=1$ and $|\bar{k}|\leq Q/2$ (first band is filled) and zero for $m>1$ (second band empty). Note that G is diagonal in $\bar{k}$ and m.

Assuming a residual interaction of the form

$$\hat{V}=\frac{1}{2}\sum_{kk'q}V_q c^{\dagger}_{k-q}c^{\dagger}_{k'+q}c_{k'}c_k , \tag{3}$$

the matrix elements for V are no longer diagonal in the momentum transfer when Eq. (3) is rewritten in the quasiparticle basis, i.e.,

$$\hat{V}=\frac{1}{2}\sum_{\bar{k}_i m_i}V_{\bar{k}_1m_1\bar{k}_2m_2\bar{k}_3m_3\bar{k}_4m_4}\Psi^{\dagger}_{\bar{k}_1m_1}\Psi^{\dagger}_{\bar{k}_2m_2}\Psi_{\bar{k}_4m_4}\Psi_{\bar{k}_3m_3} , \tag{4}$$

with

$$V_{\bar{k}_1m_1\cdots\bar{k}_4m_4}=\sum_t V(\bar{q}+tQ)g_t^{m_1m_3}(\bar{k}_1,\bar{q})g_t^{m_4m_2}(\bar{k}_4,\bar{q}) \times\delta(\bar{k}_1+\bar{k}_2-\bar{k}_3-\bar{k}_4) , \tag{5}$$

$$\bar{q}=\bar{k}_3-\bar{k}_1=\bar{k}_2-\bar{k}_4 ,$$
$$g_t^{m_1m_3}(\bar{k}_1,\bar{q})=\sum_r \alpha_r^{m_1}(\bar{k}_1)\alpha_{r+t}^{m_3}(\bar{k}_1+\bar{q}) .$$

While, from Eq. (2), the bare quasiparticle quasihole propagator is diagonal, i.e.,

$$F^0_{24,31}(\omega)=\left\{\frac{n_1^0(1-n_3^0)}{\omega-\omega_{m_3}(\bar{k}_3)+\omega_{m_1}(\bar{k}_1)+i0}-\frac{n_3^0(1-n_1^0)}{\omega-\omega_{m_3}(\bar{k}_3)+\omega_{m_1}(\bar{k}_1)-i0}\right\}\delta_{14}\delta_{23} , \tag{6}$$

the interaction renders the RPA propagator nondiagonal, viz.,

$$F_{24,31}(\omega) = F^0_{24,24}\delta_{14}\delta_{32} + F^0_{24,24}\sum_{56} V_{5264}F_{65,31} \ , \tag{7}$$

where Eq. (5) is used for V and the labels 1–4 stand for $\bar{k}_1 m_1$ to $\bar{k}_4 m_4$.

The energies of the collective modes are the pole positions of F. From Eq. (7) we find these from the zeros of the determinant of the matrix

$$H_{tt'} = \delta_{tt'} - K_{tt'}(\omega,\bar{q}) \ ,$$

with

$$K_{tt'} = V(\bar{q}+t'Q)\sum_{m_1 m_3}\int d\bar{k}\, g_t^{m_1 m_3}(\bar{k},\bar{q}) \times g_{t'}^{m_1 m_3}(\bar{k},\bar{q}) F^0_{31,31}(\omega) \ , \tag{8}$$

where $\bar{k}$ and $\bar{k}+\bar{q}$ are associated with labels 1 and 3, respectively.

The most important contribution to this expression originates from excitations between the first and second bands; we therefore extend the sum only over these two bands. A physically less obvious simplification is the assumption that the "form factors" $g_t^{m_1 m_3}$ are weakly dependent on $\bar{k}$ and can be taken out of the integral. There is strong numerical evidence that this is in fact the case: the more pronounced the band structure, the weaker the $\bar{k}$ dependence of the g_t. With these simplifications we find

$$\det(H) = 1 - \sum_t V(\bar{q}+tQ)[g_t^{1,2}(\tilde{k},\bar{q})]^2 \cdot \Pi^0_{1,2}(\omega,\bar{q}) \ , \tag{9}$$

where $\tilde{k}$ denotes an appropriate mean value and

$$\Pi^0_{1,2}(\omega,\bar{q}) = \frac{1}{2\pi}\int_{|\bar{k}|\leq k_F} d\bar{k}\left[\frac{n^0_1(1-n^0_2)}{\omega+\omega_1(\bar{k})-\omega_2(\bar{k}+\bar{q})+i0} - \frac{n^0_2(1-n^0_1)}{\omega+\omega_1(\bar{k})-\omega_2(\bar{k}+\bar{q})-i0}\right] \ . \tag{10}$$

Since Eq. (10) is just the bare polarization for the quasiparticle quasihole pair, Eq. (9) is, in a formal sense, perfectly analogous to the usual RPA in an infinite system; here, $V(q)$ is replaced by an effective interaction which has the same sign but is attenuated by $(g_t)^2$. The essential difference of the roots of Eq. (9) originates from $\Pi^0_{1,2}(\omega,\bar{q})$.

The integral in Eq. (10) can be evaluated if analytic expressions for $\omega_1(\bar{k})$ and $\omega_2(\bar{k})$ are available. While this is not exactly the case, we may approximate reasonably well the values found by computation[4] using the parametrization

$$\begin{aligned}\omega_1(\bar{k}) &= -D/2 - A\cos(2\pi\bar{k}/Q) \ ,\\ \omega_2(\bar{k}) &= D/2 + B\cos(2\pi\bar{k}/Q) \ ,\end{aligned} \tag{11}$$

with $B > A > 0$ and $D > A+B$. Inserting these Eq. (10) we obtain by contour integration

$$\Pi^0_{1,2}(\omega,\bar{q}) = \frac{Q}{2\pi}\times\begin{cases}\pm\dfrac{1}{[(\omega-D)^2-C^2]^{1/2}} \mp \dfrac{1}{[(\omega+D)^2-C^2]^{1/2}} & \text{for } \begin{matrix}\omega > D+C\\ \omega < -D-C\end{matrix}\\[2ex] -\dfrac{1}{[(\omega-D)^2-C^2]^{1/2}} - \dfrac{1}{[(\omega+D)^2-C^2]} & \text{for } |\omega| < D-C\end{cases} \ ,$$

$$C^2 = A^2+B^2+2AB\cos(2\pi\bar{q}/Q) \ . \tag{12}$$

This function is sketched in Fig. 1. It looks very different from the corresponding expression for plane waves. The new important feature is that Π^0 assumes negative real values for $|\omega| < D-C$. The determinant in Eq. (9) can therefore have zeros in that zone if $V(q)$ is negative and if

$$\left|\sum_t V(\bar{q}+Qt)|g_t^{1,2}(\bar{q})|^2\right| < \frac{4\pi(D^2-C^2)^{1/2}}{Q} \ . \tag{13}$$

Collective quasiparticle quasihole modes can therefore occur for an attractive interaction due to the energy gap of the quasiparticle spectrum which characterizes the new ground state. It is expected that this mode remains stable even when the interaction strength is increased, since D also increases while C decreases when the interaction becomes more attractive.[4]

For small values of $\bar{q}$ we expect a linear dispersion law for the eigenmode, viz.,

$$\omega_{\text{coll}}(\bar{q}) = \omega_{\text{coll}}(0) + O(\bar{q}) \ .$$

Note that the linear term originates from the effective interaction, i.e., from the terms $(g_t)^2$, since

$$g_t(\bar{q}) = (1-\delta_{t0})g_t(0) + O(\bar{q}) \ .$$

Hence, even if $V(q)$ were q independent, a linear dispersion law would occur. The precise slope of the linear term depends of course on the actual form of the interaction. Note that the polarization term [Eq. (12)] does not contribute to the linear term since

$$\Pi^0_{1,2}(\omega,\bar{q}) = \Pi^0_{1,2}(\omega,0) + O(\bar{q}^2) \ .$$

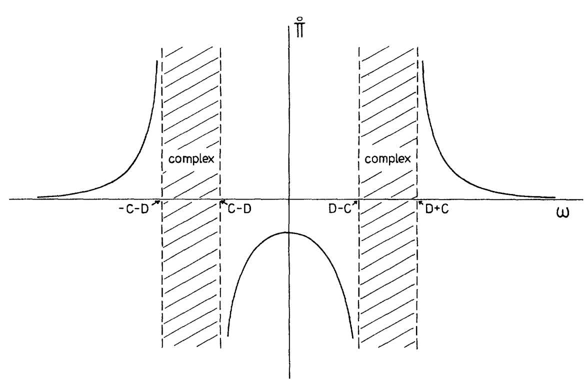

FIG. 1. The bare polarization as a function of ω and fixed momentum transfer $\bar{q}$. No qualitative change is caused when a different value is taken for $\bar{q}$.

We interpret the stability of the RPA as an indication that the new ground state which has the lattice structure is dynamically stable; this is further supported by its lower total energy. The modified Hartree-Fock ground state is, as always, only an approximation to the exact ground state and the question arises whether a linearization procedure can do justice to a dramatic change such as that occurring in a phase transition. This question was thoroughly discussed using a soluble model.[5] It appears, that, while Hartree-Fock and RPA are not reliable in the vicinity of that interaction strength for which the phase transition occurs, it can be reliably used beyond that interaction strength as was done in this paper. Note that our treatment would in fact break-down for decreasing interaction strength, since then the band structure of the single particle spectrum disappears. It appears that deformed nuclei as well as superconducting nuclei can be dealt with in an analogous fashion. These cases are being investigated.

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