Collective modes of the one-dimensional Fermi gas within the quasiparticle random-phase approximation

T. Alm

Max-Planck-Gesellschaft, AG "Theoretische Vielteilchenphysik" an der Universität Rostock, Universitätsplatz 1, D-18051 Rostock, Germany

P. Schuck

Institut des Sciences Nucléaires-IN2P3, Université Joseph Fourier, 53 avenue des Martyrs, F-38026 Grenoble Cedex, France (Received 24 October 1995; revised manuscript received 7 March 1996)

The one-dimensional Fermi gas with attractive δ interaction is treated in the quasiparticle random-phase approximation at zero temperature. The collective modes are evaluated numerically in the high-density (weak-coupling) and in the low-density (strong-coupling) case. Whereas in the weak-coupling limit the ordinary (particle-hole) random-phase approximation is approached for low momenta, the collective mode in the strong-coupling limit reproduces the Bogoliubov mode for the weakly interacting gas of particle-particle pairs (bosons). We find a smooth evolution of the collective modes from weak to strong coupling. Analytical approximations for the dispersion relation in the long-wavelength limit are derived for both weak and strong coupling. [S0163-1829(96)04728-5]

I. INTRODUCTION

The one-dimensional Fermi gas with an attractive pointinteraction among the fermions has often been used as a model system for realistic Fermi systems for several reasons.

- (i) The exact solution for its ground-state energy is known from the Bethe ansatz, so one can test approximate solutions for this system. This has been done for mean-field approximations [plane-wave Hartree-Fock (HF), non-plane-wave HF, and BCS] by Quick, Esebagg, and de Llano.² They found that the BCS solution can describe the crossover between weak coupling (a weakly interacting gas of fermions) and strong coupling (a gas of bosonic two-particle pairs) in the system. In particular, they found that the BCS solution for the ground-state energy coincides with the exact solution in both weak and strong coupling. Thus the system may serve as a simple model to study the transition between weak- and strong-coupling superconductivity in a onedimensional (1D) Fermi system. This transition between weak and strong coupling has been discussed by Leggett³ and by Nozières and Schmitt-Rink⁴ in three dimensions.
- (ii) The simple form of the interaction allows one to carry out approximations beyond the mean-field level such as ordinary random-phase approximations (RPA's) or generalized RPA's in a controlled fashion. Thus one is able to calculate contributions to the ground-state energy of the system beyond the mean-field ground-state energy. The ordinary (particle-hole) RPA for the one-dimensional electron gas was discussed by Williams and Bloch⁵ and by Brenner and Haug.⁶ The Singwi-Sjolander generalization of the ordinary RPA has been applied to the 1D electron gas by Friesen and Bergersen.⁷
- (iii) This model may serve as an initial approximation to realistic systems such as quasi-one-dimensional metals. For a review of these systems see Ref. 8.

Within this paper we will calculate the collective excitations for the 1D attractive Fermi gas with a δ interaction at

T=0 by applying the quasiparticle RPA (also known as the generalized RPA). One of the aims of the present work is to find out the limits of this perturbative approach. Furthermore, our investigation is motivated by the fact that the normal RPA in one dimension breaks down with increasing coupling, indicating an instability of the HF ground state. Moreover, even for very weak coupling the so-called Peierls instability characteristic for 1D occurs, which leads to imaginary eigenvalues in the vicinity of wave numbers $q = 2k_F$. In contrast, we will demonstrate that the quasiparticle RPA gives real solutions for all couplings. In particular, it yields the Bogoliubov sound mode for the weakly interacting boson gas in the extreme strong coupling, where the relevant degrees of freedom are two-particle bound states. Thus it is of interest to follow the evolution of the collective modes in one dimension between these two physically quite distinct limits.

We will derive the quasiparticle RPA equations for the two-quasiparticle propagators starting from the Bogoliubov transformed Hamiltonian of the system and using the equations of motion for the two-quasiparticle Green's functions. The homogeneous two-particle equations yield the condition for the collective excitations in the system, which can be given in a closed form. It coincides with the result found by Anderson, ¹⁰ Rickayzen, ¹¹ and Bardasis and Schrieffer ¹² with the equation of motion method.

This condition is evaluated numerically together with the BCS gap and density over the whole range from weak to strong coupling. A smooth transition is found for the behavior of the collective modes between these two limits. We demonstrate that the soft mode at $q = 2k_F$ (Peierls instability) characteristic for the ordinary RPA in one dimension is avoided in the quasiparticle RPA, which yields real eigenvalues for all q over the whole density range. We derive analytical approximations in the long-wavelength limit for weak and for strong coupling that are consistent with the numerical results. In particular, we can show thereby that the strong-

coupling limit of the quasiparticle RPA excitations yields the Bogoliubov dispersion relation for the weakly interacting Bose gas of two-particle pairs.

Related results for the attractive Hubbard model in two and three dimensions were derived by Sofo, Balseiro, and Castillo, ¹³ Kostyrko and Micnas, ¹⁴ Alexandrov and Rubin, ¹⁵ and Belkhir and Randeria. ¹⁶ For a review for the application to the high- T_c superconductors see Ref. 17. The quasiparticle RPA has also been applied to the problem of exciton condensation on highly excited semiconductors by Nozières and Comte¹⁸ and Cote and Griffin. ¹⁹

II. QUASIPARTICLE RPA EQUATIONS

Our starting point is the Hamiltonian for a onedimensional Fermi gas, which is given in a second quantization as

$$H = \sum_{k} \epsilon_{k} a_{k}^{\dagger} a_{k} + \frac{1}{4} \sum_{k_{1}, k_{2}, k_{3}, k_{4}} \langle k_{1} k_{2} | \overline{V} | k_{3} k_{4} \rangle a_{k_{1}}^{\dagger} a_{k_{2}}^{\dagger} a_{k_{4}} a_{k_{3}},$$

$$\tag{1}$$

where the k_i denote momentum and spin quantum number of the particles and $\langle k_1k_2|\bar{V}|k_3k_4\rangle$ is the antisymmetrized matrix element of the two-body interaction. Within this paper we will transform the Hamiltonian (1) using the Bogoliubov transformation for the creation and annihilation operators. The transformed Hamiltonian has been derived by several authors. $^{20-22}$ It can be cast in the form

$$\begin{split} H &= H^{0} + \sum_{k_{1},k_{2}} H^{11}_{k_{1},k_{2}} \alpha^{\dagger}_{k_{1}} \alpha_{k_{2}} + \frac{1}{2} \sum_{k_{1},k_{2}} \left(H^{20}_{k_{1}k_{2}} \alpha^{\dagger}_{k_{1}} \alpha^{\dagger}_{k_{2}} + \text{H.c.} \right) \\ &+ \sum_{k_{1},k_{2},k_{3},k_{4}} \left(H^{40}_{k_{1}k_{2}k_{3}k_{4}} \alpha^{\dagger}_{k_{1}} \alpha^{\dagger}_{k_{2}} \alpha^{\dagger}_{k_{3}} \alpha^{\dagger}_{k_{4}} + \text{H.c.} \right) \\ &+ \sum_{k_{1},k_{2},k_{3},k_{4}} \left(H^{31}_{k_{1}k_{2}k_{3}k_{4}} \alpha^{\dagger}_{k_{1}} \alpha^{\dagger}_{k_{2}} \alpha^{\dagger}_{k_{3}} \alpha_{k_{4}} + \text{H.c.} \right) \\ &+ \frac{1}{4} \sum_{k_{1},k_{2},k_{3},k_{4}} H^{22}_{k_{1}k_{2}k_{3}k_{4}} \alpha^{\dagger}_{k_{1}} \alpha^{\dagger}_{k_{2}} \alpha_{k_{4}} \alpha_{k_{3}}. \end{split} \tag{2}$$

In Eq. (2) H^0 is the BCS ground-state energy and the diagonal part H^{11} is given by

$$H_{k_{1},k_{2}}^{11} = \left[\left(\epsilon_{k_{1}} - \mu \right) \delta_{k_{1},k_{2}} + \frac{1}{2} \langle k_{1}k_{2} | \overline{V} | k_{1}k_{2} \rangle v_{k_{2}}^{2} \right] \left[u_{k_{1}}^{2} - v_{k_{1}}^{2} \right]$$

$$+ 2 \langle k_{1} - k_{1} | \overline{V} | k_{2} - k_{2} \rangle u_{k_{1}} v_{k_{1}} u_{k_{2}} v_{k_{2}}.$$
 (3)

The off-diagonal part H^{20} is given by

$$\begin{split} H_{k_{1},k_{2}}^{20} = & 2[(\epsilon_{k_{1}} - \mu)\delta_{k_{1},k_{2}} + \frac{1}{2}\langle k_{1}k_{2}|\bar{V}|k_{1}k_{2}\rangle v_{k_{2}}^{2}]u_{k_{1}}v_{k_{1}} \\ & - \langle k_{1} - k_{1}|\bar{V}|k_{2} - k_{2}\rangle (u_{k_{1}}^{2} - v_{k_{1}}^{2})u_{k_{2}}v_{k_{2}}. \end{split} \tag{4}$$

If one demands the off-diagonal part H^{20} (4) to vanish, this yields the BCS, gap equation and the well-known relations for u_k and v_k

$$u_k^2 = 1 - v_k^2 = \frac{1}{2} \left[1 + \frac{\xi_k}{E_k} \right].$$
 (5)

where $\xi_k = \epsilon_k + V_k^{\rm HF} - \mu$ and the BCS quasiparticle energy is given as $E_k = \sqrt{\xi_k^2 + \Delta_k^2}$. The H^{31} term in the Hamiltonian is given, e.g., in Ref. 22; however, it does not contribute to the RPA equations.

The remaining terms in the Hamiltonian describe the residual interaction among the BCS quasiparticles. They are given by 21,22

$$H_{k_{1}k_{2}k_{3}k_{4}}^{40} = \frac{1}{4!} \left[-\langle k_{1}k_{2}|\overline{V}| - k_{3} - k_{4} \rangle (u_{k_{1}}u_{k_{2}}v_{k_{3}}v_{k_{4}} + v_{k_{1}}v_{k_{2}}u_{k_{3}}u_{k_{4}}) + \langle k_{1}k_{3}|\overline{V}| - k_{2} - k_{4} \rangle \right.$$

$$\times (u_{k_{1}}v_{k_{2}}u_{k_{3}}v_{k_{4}} + v_{k_{1}}u_{k_{2}}v_{k_{3}}u_{k_{4}})$$

$$+ \langle k_{3}k_{2}|\overline{V}| - k_{1} - k_{4} \rangle$$

$$\times (u_{k_{1}}v_{k_{3}}v_{k_{2}}u_{k_{3}} + v_{k_{1}}u_{k_{2}}u_{k_{3}}v_{k_{4}}) \right], \tag{6}$$

$$\begin{split} H_{k_{1}k_{2}k_{3}k_{4}}^{22} &= [-\langle k_{1}k_{2}|\overline{V}|k_{3}k_{4}\rangle(u_{k_{1}}u_{k_{2}}u_{k_{3}}u_{k_{4}} + v_{k_{1}}v_{k_{2}}v_{k_{3}}v_{k_{4}}) \\ &-\langle k_{1}-k_{3}|\overline{V}|k_{4}-k_{2}\rangle(u_{k_{1}}v_{k_{2}}v_{k_{3}}u_{k_{4}} \\ &+ v_{k_{1}}u_{k_{2}}u_{k_{3}}v_{k_{4}}) + \langle k_{2}-k_{3}|\overline{V}|k_{4}-k_{1}\rangle \\ &\times (v_{k_{1}}u_{k_{2}}v_{k_{3}}u_{k_{4}} + u_{k_{1}}v_{k_{2}}u_{k_{3}}v_{k_{4}})]. \end{split}$$

These terms are neglected in the usual BCS approximation. However, in order to go beyond the BCS mean-field approximation it is necessary to include the residual interaction among the quasiparticles.

Within this section the quasiparticles will be treated within the generalized RPA approximation. We introduce two-particle Green's function with respect to the quasiparticle basis as

$$\begin{pmatrix} G^{11} & G^{12} \\ G^{21} & G^{22} \end{pmatrix}_{k_1 k_2 k_3 k_4}^{t-t'}$$

$$=i\left(\begin{array}{ccc} \left\langle T(\alpha_{k_1}\alpha_{k_2})_t(\alpha_{k_3}^\dagger\alpha_{k_4}^\dagger)_{t'}\right\rangle & \left\langle T(\alpha_{k_1}\alpha_{k_2})_t(\alpha_{k_3}\alpha_{k_4})_{t'}\right\rangle \\ \left\langle T(\alpha_{k_1}^\dagger\alpha_{k_2}^\dagger)_t(\alpha_{k_3}^\dagger\alpha_{k_4}^\dagger)_{t'}\right\rangle & \left\langle T(\alpha_{k_1}^\dagger\alpha_{k_2}^\dagger)_t(\alpha_{k_3}\alpha_{k_4})_{t'}\right\rangle \end{array}\right), \tag{8}$$

where $(a)_t = e^{iHt}a(0)e^{-iHt}$. As shown in Ref. 23, one can derive an approximation for the equation of motion for this matrix Green's function **G** in the form

$$i \frac{d}{dt} \mathbf{G}_{\mathbf{k}_{1} \mathbf{k}_{2} \mathbf{k}_{3} \mathbf{k}_{4}, \mathbf{t} - \mathbf{t}'}$$

$$= \delta(\mathbf{t} - \mathbf{t}') \, \delta_{\mathbf{k}_{1}, \mathbf{k}_{3}} \delta_{\mathbf{k}_{2}, \mathbf{k}_{4}} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$+ \begin{pmatrix} (E_{k_{1}} + E_{k_{2}}) \, \delta_{k_{1}, k_{3}} \, \delta_{k_{2}, k_{4}} & 0 \\ 0 & -(E_{k_{1}} + E_{k_{2}}) \, \delta_{k_{1}, k_{3}} \, \delta_{k_{2}, k_{4}} \end{pmatrix}$$

$$\times \mathbf{G}_{k_{3}' k_{4}' k_{3} k_{4}, t - t'}$$

$$+ \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \sum_{k_{3}', k_{4}'} \begin{pmatrix} \widetilde{A}_{k_{1} k_{2} k_{3}' k_{4}'} & B_{k_{1} k_{2} k_{3}' k_{4}'} \\ -B_{k_{1} k_{2} k_{3}' k_{4}'} & -\widetilde{A}_{k_{1} k_{2} k_{3}' k_{4}'} \end{pmatrix}$$

$$\times \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \mathbf{G}_{k_{3}' k_{4}' k_{3} k_{4}, t - t'}. \tag{9}$$

Equation (9) has the form of a Dyson equation for the two-particle propagator matrix G, where the static elements of the mass operator \widetilde{A} and B are given by the double commutators²⁴

$$\widetilde{A}_{k_{1}k_{2}k_{3}k_{4}} = A_{k_{1}k_{2}k_{3}k_{4}} - (E_{k_{1}} + E_{k_{2}}) \, \delta_{k_{1},k_{3}} \delta_{k_{2},k_{4}},$$

$$A_{k_{1}k_{2}k_{3}k_{4}} = \langle [\alpha_{k_{1}}\alpha_{k_{1}}, [H, \alpha_{k_{2}}^{\dagger}, \alpha_{k_{4}}^{\dagger}]] \rangle,$$
(10)

and

$$B_{k_1 k_2 k_3 k_4} = -\langle [\alpha_{k_2} \alpha_{k_1}, [H, \alpha_{k_4} \alpha_{k_3}]] \rangle. \tag{11}$$

In our case $\langle \, \rangle$ means averaging with respect to the BCS ground state. However, if instead of the BCS ground state an approximation to the correlated ground state is used, this corresponds to a generalized quasiparticle RPA (see Ref. 25 for details). The double commutation with respect to the Hamiltonian (2) can be carried out with the result:²²

$$\widetilde{A}_{k_1 k_2 k_3 k_4} = H_{k_1 k_2 k_3 k_4}^{22} \tag{12}$$

and

$$\widetilde{B}_{k_1 k_2 k_3 k_4} = 4! H_{k_1 k_2 k_3 k_4}^{40}, \tag{13}$$

where the expressions for H^{40} and for H^{22} are given by Eqs. (6) and (7).

For the δ interaction under consideration it is possible to solve the system of equations in the ω representation algebraically. This will be demonstrated for the coupled equations for G^{11} and G^{21} (G^{22} and G^{12} can be treated analogously). Introducing relative coordinates for the momenta and omitting the spin indices, the corresponding equations read

$$G^{11}(kk'q,\omega) = G_0^{11}(kq,\omega) \, \delta_{k,k'}$$

$$+ G_0^{11}(kq,\omega) \sum_{k''} \, \widetilde{A}_{kk''q} G_{11}(k''k'q,\omega)$$

$$- G_0^{11}(kq,\omega) \sum_{k''} \, B_{kk''q} G^{21}(k''k'q,\omega), \qquad (14)$$

$$G^{21}(kk'q,\omega) = G_0^{22}(kq,\omega) \sum_{k''} \, B_{kk''q} G^{11}(k''k'q,\omega)$$

$$- G_0^{22}(kq,\omega) \sum_{k''} \, \widetilde{A}_{kk''q} G^{21}(k''k'q,\omega), \qquad (15)$$

where $G_0^{11}(kq,\omega)=1/(\omega-E_{k,q}), \quad G_0^{22}(kq,\omega)=1/(\omega+E_{k,q}),$ and $E_{k,q}=E_k+E_{k+q}$. An analogous coupled system is found for G^{22} and G^{12} . Adding and subtracting Eqs. (14) and (15), taking into account that the matrix elements for our model are constants in momentum space, i.e., $\langle k_1k_2|\overline{V}|k_3k_4\rangle=v\,\delta_{k_1+k_2,k_3+k_4}(\delta_{\sigma_1,\sigma_3}\delta_{\sigma_2,\sigma_4}-\delta_{\sigma_1,\sigma_4}\delta_{\sigma_2,\sigma_3}),$ and assuming that the collective pairs have zero total spin (see also Ref. 21), we arrive at the expressions

$$G^{11}(kk'q,\omega) + G^{21}(kk'q,\omega)$$

$$= G_0^{11}(kq,\omega) \,\delta_{k,k'} + \frac{1}{\omega^2 - E_{k,q}^2} \left[2E_{k,q}m(k,q)Z_{k',q,\omega} + E_{k,q}n(k,q)\Lambda_{k',q,\omega} + \omega l(k,q)\Gamma_{k',q,\omega} \right]$$
(16)

and

$$G^{11}(kk'q,\omega) - G^{21}(kk'q,\omega)$$

$$= G_0^{11}(kq,\omega) \, \delta_{k,k'} + \frac{1}{\omega^2 - E_{k,q}^2} \left[2\,\omega m(k,q) Z_{k',q,\omega} + \omega n(k,q) \Lambda_{k',q,\omega} + E_{k,q} l(k,q) \Gamma_{k',q,\omega} \right]. \tag{17}$$

The quantities Z, Λ , and Γ are given by the equations

$$Z_{k,q,\omega} = -\frac{v}{2} \sum_{k''} m(k'',q) [G^{11}(k''kq,\omega) + G^{21}(k''kq,\omega)],$$
(18)

$$\Lambda_{k,q,\omega} = -v \sum_{k''} n(k'',q) [G^{11}(k''kq,\omega) + G^{21}(k''kq,\omega)],$$
(19)

$$\Gamma_{k,q,\omega} = -v \sum_{k''} l(k'',q) [G^{11}(k''kq,\omega) - G^{21}(k''kq,\omega)]$$
(20)

and the m(k,q), n(k,q), and l(k,q) are combinations of u_k and v_k , given by

$$m(k,q) = u_k v_{k+q} + v_k u_{k+q},$$
 (21)

$$n(k,q) = u_k u_{k+q} - v_k v_{k+q}, \qquad (22)$$

$$l(k,q) = u_k u_{k+q} + v_k v_{k+q}. (23)$$

Multiplying in Eq. (16) subsequently with m with n and in Eq. (17) with l and summing over k, we arrive at the system of equations for the quantities Z, Λ , and Γ ,

$$\begin{pmatrix} 1 + vI_{E,n,n}(q,\omega) & vI_{\omega,n,l}(q,\omega) & 2vI_{E,n,m}(q,\omega) \\ vI_{\omega,n,l}(q,\omega) & 1 + vI_{E,l,l}(q,\omega) & 2vI_{\omega,l,m}(q,\omega) \\ v/2I_{E,n,m}(q,\omega) & v/2I_{\omega,l,m}(q,\omega) & 1 + vI_{E,m,m}(q,\omega) \end{pmatrix} \times \begin{pmatrix} \Lambda \\ \Gamma \\ Z \end{pmatrix}_{k,q,\omega} = \begin{pmatrix} -vn(k,q)G_0^{11} \\ -vl(k,q)G_0^{11} \\ -v/2m(k,q)G_0^{11} \end{pmatrix}. \tag{24}$$

The quantities $I_{a,b,c}$ are in the notation of Ref. 16, given by

$$I_{a,b,c} = \sum_{k} \frac{a(k,q)b(k,q)c(k,q)}{\omega^2 - E_{k,q}^2},$$
 (25)

with $a(k,q) = [E_{k,q}, \omega]$ and b(k,q), c(k,q) = [n(k,q), l(k,q), m(k,q)]. This is a linear inhomogeneous system of equations for the quantities Λ , Γ , and Z, which can be solved easily by matrix inversion. With the solution for these quantities the elements of the Green's function matrix are given by (16) and (17) and the corresponding equations for G^{22} and G^{12} . In the homogeneous case, i.e., if the right-hand side of the equation vanishes, Eq. (24) is an eigenvalue problem for the determination of the collective modes in the quasiparticle RPA. The condition for a nontrivial solution is the vanishing of the determinant

$$\begin{vmatrix} 1+vI_{E,n,n}(q,\Omega) & vI_{\Omega,n,l}(q,\Omega) & 2vI_{E,n,m}(q,\Omega) \\ vI_{\Omega,n,l}(q,\Omega) & 1+vI_{E,l,l}(q,\Omega) & 2vI_{\Omega,l,m}(q,\Omega) \\ v/2I_{E,n,m}(q,\Omega) & v/2I_{\Omega,l,m}(q,\Omega) & 1+vI_{E,m,m}(q,\Omega) \end{vmatrix} = 0,$$
 (26)

where $\Omega(q)$ denotes the eigenvalue for the collective excitations. An analogous condition to (26) for the collective modes in the Hubbard model has also been derived by Belkhir and Randeria¹⁶ using the equation of motion method of Bardasis and Schrieffer.¹²

The elements of the coefficient matrix in Eq. (24) can be interpreted as generalizations of the well-known Lindhard function of the ordinary RPA. In particular, the element $I_{E,m,m}(q,\omega)$ is the generalization of the one-dimensional Lindhard function of the ordinary particle-hole RPA, which it approaches in the limit $\Delta \to 0$. The elements $I_{E,n,n}(q,\omega)$, $I_{E,l,l}(q,\omega)$, and $I_{\omega,n,l}(q,\omega)$ constitute the corresponding generalization of the particle-particle (hole-hole) RPA. All the other elements of the matrix represent couplings between the particle-hole and the particle-particle channel and consequently vanish in the limit $\Delta \to 0$. In short, we see that in the nonsuperconducting limit we recover the well-known particle-hole and particle-particle (hole-hole) branches separately. As has already been noted in Ref. 16, in the limit $q\to 0$ the element $1+vI_{E,l,l}(q=0,\omega=0)$ yields the BCS gap equation.

In the next subsection we will discuss the behavior of the collective modes from the numerical solution of Eq. (26) as well as analytically in certain limiting cases.

III. THE COLLECTIVE MODE SPECTRUM IN THE GENERALIZED RPA

According to the preceding subsection, the collective modes for a contact interaction are given by the solution of Eq. (26). Before discussing the numerical solution for the collective modes, we will derive analytical expressions for small q and Ω .

A. Weak-coupling case

The analysis of the weak-coupling case has already been given by Belkhir and Randeria. ¹⁶ We quote their result for the weak-coupling collective mode in one dimension:

$$\Omega(q) = \left[1 - v \, \frac{1}{\pi} \, \frac{m}{k_F}\right]^{1/2} \frac{k_F}{m} \, q,\tag{27}$$

where the density of states in one dimension for the parabolic dispersion was used. For the details of the expansion we refer to Ref. 16. Thus the long-wavelength collective modes in the weak-coupling case have a phononlike spectrum and are independent of the gap. If one compares Eq. (27) with the small-q expansion of the collective modes in the particle-hole RPA, one finds that both coincide. This means that in weak coupling the behavior of the collective modes for small q is not changed from the normal particle-hole RPA.

However, for large q and in particular near the point $q=2k_F$, the quasi-particle RPA differs from the particle-hole RPA qualitatively. Due to the presence of a finite gap the continuum does not reach zero at $q=2k_F$ as it does in the particle-hole RPA case. This means that the imaginary eigenvalues at this particular energy typical for the particle-hole RPA do not necessarily show up in the generalized RPA. In fact, as will be shown below by our numerical evaluation, imaginary eigenvalues no longer appear at any coupling in the quasiparticle RPA. However, in the high-density (weak-coupling) limit the tendency of the system towards the for-

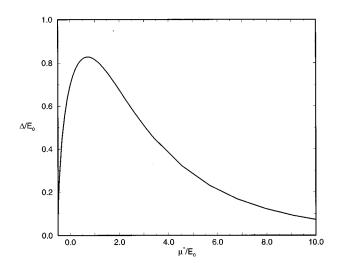


FIG. 1. BCS gap parameter Δ as a function of the effective chemical potential μ^* for a fixed coupling strength $v/(2\pi)=0.3$. Both quantities are given in units of the two-particle binding energy in the vacuum E_0 .

mation of density waves remains, as indicated by a pronounced minimum of $\Omega(q)$ at $q = 2k_F$ (see below).

B. Strong-coupling case

In Ref. 16 the strong-coupling case is treated for the Hubbard model. Here we will derive expressions for the strong-coupling case for the continuum model under consideration. In the extreme strong-coupling limit the gap goes to zero with the density. Thus we will start from an expansion of the determinant for the collective modes (26) (in the small-q and - Ω limit) with respect to a small gap. As a first step we expand the gap equation in terms of Δ^2 ,

$$1 = \frac{v}{2\pi} \int_0^\infty dk \, \frac{1}{|\xi_k| \left(1 + \frac{\Delta^2}{|\xi_k|^2}\right)^{1/2}}$$

$$\approx \frac{v}{2\pi} \int_0^\infty dk \, \frac{1}{|\xi_k|} - v \, \frac{\Delta^2}{4\pi} \int_0^\infty dk \, \frac{1}{|\xi_k|^3}$$

$$= \frac{v}{2\pi} J_1 - \frac{v \Delta^2}{4\pi} J_3. \tag{28}$$

It is interesting to note that the integral in the first line of Eq. (28) is convergent for a contact interaction without a cutoff due to the one dimensionality of the system. An analogous expansion of the BCS density equation yields

$$n = \frac{1}{\pi} \int_0^\infty dk \ 1 - \frac{1}{|\xi_k| \left(1 + \frac{\Delta^2}{|\xi_k|^2}\right)^{1/2}}$$

$$\approx \frac{1}{2\pi} \Delta^2 \int_0^\infty dk \ \frac{1}{|\xi_k|^2} = \frac{1}{2\pi} \Delta^2 J_2, \tag{29}$$

where $\xi_k = k^2/2m - \mu^*$ and μ^* is the effective chemical potential including the quasiparticle shift. The integrals J_i are given in the Appendix. With the help of these expansions, the effective chemical potential can be expressed in terms of the density and the coupling strength as

$$|\mu^*|^{1/2} = \frac{\sqrt{2}}{8} m^{1/2} v \pm \sqrt{\frac{2}{64} m v^2 - \frac{3}{8} n v}.$$
 (30)

In the limit of zero density or zero gap, respectively, Eq. (30) yields the condition

$$2|\mu^*| = \frac{mv^2}{4} = E_0. \tag{31}$$

This means that in the extreme strong-coupling limit the chemical potential, i.e., the energy to remove a particle from the system, is just half the two-particle binding energy $-E_0$ in the vacuum.²

As a next step we carry out an expansion of the elements of the determinant (26) for small q and Ω . In the weak-coupling case considered in Ref. 16, it is sufficient to consider the elements $1+I_{E,l,l}$, $1+I_{E,m,m}$, and $I_{\Omega,l,m}$ only. However, in order to treat the strong-coupling limit we carried out the expansion for the other elements $1+I_{E,n,n}$, $I_{E,n,m}$, and $I_{\Omega,n,l}$ in Eq. (26) as well. After this expansion the approximate expression for the determinant (26) reads

$$\begin{vmatrix} 1 - \frac{v}{2} r & -\frac{v}{4} t\Omega & -v \Delta t \\ -\frac{v}{4} t\Omega & \frac{v}{8} \left[(3z + \overline{w} - y)q^2 - x\Omega^2 \right] & \frac{v}{2} \Delta x\Omega \\ -\frac{v}{4} \Delta t & \frac{v}{8} \Delta x\Omega & 1 - \frac{v}{2} \Delta^2 x \end{vmatrix} = 0.$$
(32)

The coefficients r,t,\overline{w},x,y,z as well as their expansion in terms of Δ^2 are given in the Appendix.

Thus the long-wavelength dispersion relation in the strong-coupling limit is given by

$$\Omega(q) = cq, \tag{33}$$

where the sound velocity c depends on the gap Δ . Using the expression (32) together with the expansions for the coefficients given in the Appendix, the sound velocity was evaluated in the lowest nonvanishing order in Δ^2 . In the next step we used the low-density expansion of the BCS density (29) to substitute Δ^2 by the density n. Moreover, we expressed the chemical potential in the integrals J_i (see the Appendix) by the interaction v using Eq. (30) (in the lowest order in n). Collecting the various terms in c, one ends up with the following simple expression for the collective modes in the strong-coupling limit:

$$\Omega(q) = \left[\frac{vn}{4m}\right]^{1/2} q. \tag{34}$$

Introducing the pair mass $m_B=2m$ and the pair density $n_B=n/2$, this expression reads

$$\Omega(q) = \left[\frac{v n_B}{m_B}\right]^{1/2} q. \tag{35}$$

The result Eq. (34) for the sound velocity can easily be verified starting from the ground-state energy in the BCS approximation (strong-coupling limit) as given in Eq. (9) of Ref. 2. This can be done using thermodynamic relations, as presented in detail in Ref. 29.

However, repeating the same derivation for the exact ground-state energy, of which the strong-coupling limit was derived in Refs. 2 and 27, one finds the following result for the velocity of sound:

$$c = \frac{\pi \hbar n}{4m},\tag{36}$$

n being the total density. Equation (36) is the exact result for the sound velocity, which is independent of the attraction strength. This is at variance with the perturbative result (34). The reason for this difference can be traced back to the fact that the BCS approximation for the ground-state energy in the strong coupling has a different behavior compared to the exact solution (see Ref. 2 for details). Thus although the BCS approximation approaches the exact expression for the ground-state energy in the limit of strong coupling $(n/v \rightarrow 0)$ derivative quantities such as the sound velocity may differ substantially from the exact solution in this limit. The inclu-

sion of correlations beyond the quasiparticle RPA (generalized RPA) is necessary in order to improve the perturbative treatment.

Equation (35) is the well-known Bogoliubov dispersion relation for the weakly interacting Bose gas^{28,29} in the limit of small q, which is linear in q, i.e., phononlike. Thus, starting from interacting Fermions with an attractive interaction, the quasiparticle RPA in the strong-coupling limit yields the dispersion relation for a weakly interacting gas of bosons (two-particle bound states). This has already been shown for the attractive Hubbard model by Belkhir and Randeria. 16 The fact that the magnitude of the repulsive interaction among the bosons in Eq. (35) is given by the fermionic interaction strength v is consistent with the results of Haussmann. ³⁰ Relating the bosonic scattering length in three dimensions a_R to the interaction among the bosons in the usual way $a_B = m_B v_B / \hbar^2 4\pi$ (Ref. 29) and $a_F = m_F v_F \hbar^2 / 4\pi$, the condition $a_R = 2a_F$ (Ref. 30) yields $v_R = v_F$. This coincides with our result in one dimension Eqs. (34) and (35). In the opposite limit of large q the strong-coupling dispersion approaches the value $\Omega = q^2/2m_B$ for noninteracting pairs.

In order to investigate the behavior of the collective modes between the two limiting cases of weak and strong coupling and within the whole q range one has to evaluate Eq. (26) numerically. We solve Eq. (26) for a fixed value of $v/(2\pi)=0.3$. With this value for v the BCS gap equation [first line in Eq. (28)] is solved to obtain the gap Δ for a given effective chemical potential μ^* (or density n, respectively).

In Fig. 1 we give the BCS gap Δ as a function of the effective chemical potential μ^* (both quantities in units of the two-particle binding energy E_0). We see that the gap starts at zero for $\mu^*=-0.5E_0$, corresponding to the density n=0 (strong coupling limit), consistent with Eq. (29). The gap has a maximum of at $\mu^*=0.5E_0$ and then gradually decreases with increasing chemical potential (density) in the weak-coupling limit. The fact that the gap will not reach zero for any finite density is due to the purely attractive interaction among the fermions.

Having solved the BCS theory, we are able to solve numerically the condition for the dispersion relation of the collective modes (26). In order to demonstrate the behavior of the collective modes if one goes from weak coupling to strong coupling we keep the interaction $v/(2\pi)=0.3$ fixed and vary the effective chemical potential (or the density respectively).

In Fig. 2(a) we present the extreme weak-coupling regime corresponding to large densities ($\mu^*=11.28E_0$). The gap in this limit is very small $\Delta=0.052~93E_0$. The numerical solution for the dispersion relation $\Omega(q)$ is given as a solid line. It starts at q=0 and is linear in q for small q values (see below). We find that the full solution (solid line) is very close to the continuum edge (dotted line) over the whole q range. The above-mentioned tendency towards the formation of density waves is signaled by the pronounced minimum at $q=2k_F$. However, due to the presence of the gap, the continuum edge does not reach zero in this case as it does in the normal particle-hole RPA. This makes it possible for the collective mode to have a real value at $q=2k_F$, which is in contrast to the normal RPA, where it has an imaginary solu-

tion at this particular q value for arbitrarily weak coupling. This is known as Peierls instability⁹ and is characteristic for the one-dimensional system.

In Fig. 2(b) the effective chemical potential is $\mu^*=3.386E_0$ and the corresponding gap $\Delta=0.4518E_0$. The distance of the collective mode to the continuum edge has increased due to the increased coupling. The behavior is still characterized by a minimum at $q=2k_F$. However, due to the larger gap (2Δ as the minimum of the continuum edge is given by the dash-dotted line), the way the finite gap prevents the collective modes from becoming soft is more clearly to be seen. This means the finite gap acts as to stabilize the BCS ground state against the formation of density waves, which always show up in the HF ground state in the corresponding particle-hole RPA.

The form of the dispersion relation in the weak- and intermediate-coupling regimes is similar to the excitation spectrum of liquid 4 He. In particular, it starts linearly for small q and it exhibits a pronounced rotorlike minimum at higher q.

In Fig. 2(c) the effective chemical potential is $\mu^*=1.1286E_0$ and the corresponding gap $\Delta=0.8038E_0$ (close to the maximum gap in Fig. 1). One observes that the behavior of the collective modes has changed compared to the weak-coupling case. There is only a very weak minimum at $q=2k_F$. The distance to the continuum edge has further increased.

In Fig. 2(d) we have reached the extreme strong-coupling limit $(\mu^*=-0.4966E_0, \Delta=0.072\ 18E_0)$. We see that no longer is there a minimum in the dispersion relation for the collective mode. Instead it is a monotonically increasing function, which approaches the free particle limit $\omega=q^2/4m$ for all except very small q values. For very small q values we have a linear behavior in q, which will be discussed below [Fig. 3(b)].

In Figs. 3(a) and 3(b) we will demonstrate that the behavior of the numerically found collective modes for small q is consistent with the corresponding expansions for weak- and strong-coupling carried out above.

In Fig. 3(a) we consider the weak-coupling case $(\mu^*=3.386E_0)$. The behavior of the numerical solution (full line) is compared to the weak-coupling expansion Eq. (27) (dashed line). Both coincide for small q, indicating the consistency of the numerical solution with the well-known weak-coupling result, which was obtained by Anderson¹⁰ in the 3D case.

In Fig. 3(b) the strong-coupling limit ($\mu^* = -0.4966E_0$) is plotted for small q. We see that indeed the full solution starts linearly in q, consistent with the strong-coupling expansion given in Eq. (35), which is plotted as a dashed line. This confirms the interpretation of the collective excitations in the strong-coupling limit as Bogoliubov sound modes of the two-particle Bose gas that is formed in this limit. Also plotted is the free-particle dispersion $q^2/2m_B$ (dash-dotted line), which is reached by the full solution for large q.

IV. SUMMARY

The equations for the quasiparticle RPA were derived using Green's function methods for the Hamiltonian in the representation by Bogoliubov quasiparticles. A condition for the

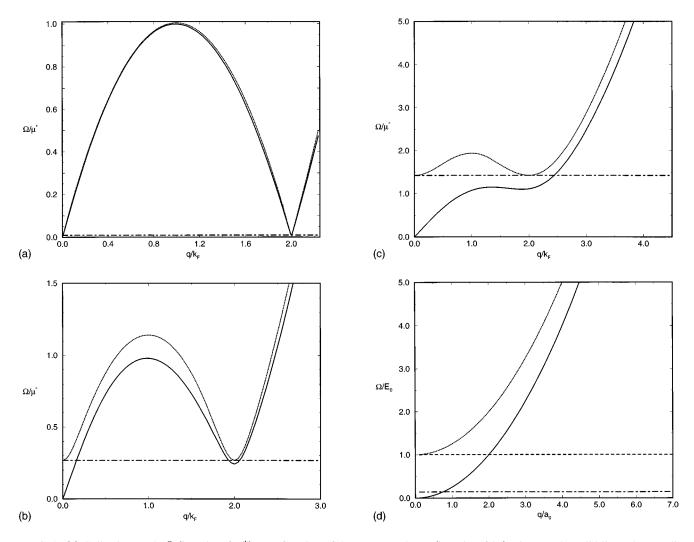


FIG. 2. (a) Collective mode Ω (in units of μ^*), as a function of the wave number q (in units of k_F), given as the solid line. The coupling strength is $v/(2\pi)=0.3$ and the effective chemical potential is $\mu^*=11.28E_0$. The continuum edge is given as a dotted line. The dash-dotted line indicates the value 2Δ as the minimal value for the continuum edge. (b) Same as in (a) but for $\mu^*=3.386E_0$. (c) Same as in (a) but for $\mu^*=1.1286E_0$. (d) Collective mode Ω as a function of the wave number q for $\mu^*=-0.4966E_0$ (solid line). The collective modes Ω are given in terms of the two-particle binding energy in the vacuum E_0 , defined in the text, and the wave number q in terms of $a_0=\sqrt{mE_0}$. The dashed line denotes the minimal value for the continuum edge, which for $\mu^*<0$ is given by $2\sqrt{\mu^{*2}+\Delta^2}$.

collective modes in one dimension was found for the case of an attractive δ interaction. Analytical approximations were derived in the long-wavelength limit for the weak- and the strong-coupling limits. In particular, we could show that in the weak-coupling limit we recover Anderson's result, 10 whereas in the strong-coupling limit the Bogoliubov dispersion relation 28 for the interacting Bose gas of two-particle pairs can be derived from the quasiparticle RPA. This is consistent with the fact that the BCS theory is capable of describing the extreme strong-coupling limit, i.e., the gas of two-particle bound states, properly and reproduces the exact result for the ground-state energy in this limit. 2

In order to study the transition from weak to strong coupling the condition for the collective modes was evaluated numerically for the whole q range. We found that the tendency of the system to form density waves is reflected in a pronounced minimum of the dispersion for $\Omega(q)$ at $q = 2k_F$ in the extreme weak-coupling (high-density) case. However, there are no imaginary eigenvalues at $q = 2k_F$ as characteristic for the normal RPA (Ref. 5) over the whole coupling

range. The finite gap stabilizes the ground state with respect to the Peierls instability. With decreasing density the minimum at $q = 2k_F$ becomes less pronounced due to the increasing gap. In the strong-coupling limit the dispersion relation changes qualitatively. It is a monotonic function of q that reproduces the $q^2/2m_B$ behavior for large q. For small q it reproduces the phononlike Bogoliubov dispersion relation of the weakly interacting Bose gas.

Summarizing, we could show that the treatment of the residual interaction in the Hamiltonian (2) within the quasiparticle or generalized RPA allows one to study the behavior of the collective modes over the whole coupling range. In particular, it yields the physically plausible result of the Bogoliubov mode for the weakly interacting Bose gas at very low densities. Thus the quasiparticle RPA, in contrast to the normal RPA, may serve as a reasonable starting point for a calculation of the ground-state energy, including the scattering part of Eq. (16). However, the comparison of our result for the sound velocity in the strong-coupling limit derived from the quasiparticle RPA with the value for the sound

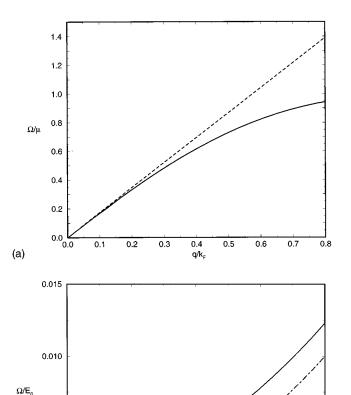


FIG. 3. (a) Collective mode Ω for small momenta q, in the weak-coupling case ($\mu^*=3.386E_0$). The numerical solution (full line) is compared to the weak-coupling expansion (27) (dashed line). (b) Collective mode Ω , for small momenta q, in the strong-coupling case ($\mu^*=-0.4966E_0$). The numerical solution (full line) is compared to the strong-coupling expansion (35) (dashed line). The free dispersion $\Omega=q^2/4m$ is also given as a dash-dotted line.

0.10

0.15

0.20

0.05

0.005

(b)

velocity derived from the exact solution for the ground-state energy is in qualitative disagreement. This demonstrates the necessity to further improve the perturbative treatment in the strong-coupling limit.

Finally, we would like to mention possible extensions of the treatment given above. Bychkov, Gorkov, and Dzyaloshinski³¹ suggested, in order to treat the Peierls instability and the Cooper singularity in a finite temperature approach on equal footing, the introduction, in addition to the BCS gap, of a so-called dielectric gap that opens at the critical temperature for the Peierls transition.

In order to improve the treatment given above at intermediate couplings it is necessary to include ground-state correlations beyond the quasiparticle RPA. Such an calculation beyond the standard RPA has recently been carried out for the Heisenberg antiferromagnet. In particular, it has been shown that for the seniority model a generalization of the quasiparticle RPA yields genuine four-particle correlations. Work in this direction is in progress.

ACKNOWLEDGMENTS

The authors wish to thank Jorge Dukelsky, Gerd Röpke, and Steffen Schäfer for stimulating discussions and valuable hints. One of the authors (Th.A.) wants to thank his colleagues at the Theory Department of ISN Grenoble for the hospitality extended to him during his stay. This work was carried out through the Deutsche Akademische Austauschdienst under Grant No. D/94/06775.

APPENDIX

In Eqs. (28), (29), and (A2) integrals J_i are introduced. They will be evaluated for the strong-coupling lines, i.e., for $\mu^* < 0$ throughout. Here we give the explicit expressions

$$J_{i} = \int_{0}^{\infty} dk \, \frac{1}{\left(\frac{k^{2}}{2m} + \left|\mu^{*}\right|\right)^{i}},$$

$$J_{i2} = \int_{0}^{\infty} dk \, \frac{k^{2}}{\left(\frac{k^{2}}{2m} + \left|\mu^{*}\right|\right)^{i}}.$$
(A1)

The integrals (A1) are easily evaluated to yield $J_1 = \pi m^{1/2}/(2|\mu^*|)^{1/2}, \ J_2 = m^{1/2}\pi/(2|\mu^*|)^{3/2}, \ J_3 = 3m^{1/2}\pi/(2|\mu^*|)^{3/2}, \ J_3 = 3m^{1/2}\pi/(2|\mu^*|)$

As the next step we will give the results for the coefficients of the elements in the determinant (32) resulting from an expansion for small q and Ω . For $1+I_{E,n,n}$, $1+I_{E,m,m}$, and $I_{\Omega,l,m}$ we quote the weak-coupling results of Ref. 16. In addition, the expansions for $1+I_{E,n,n}$, $I_{\Omega,n,l}$, and $I_{E,n,m}$ necessary for strong coupling are given. These coefficients are then evaluated to order Δ^2 :

$$r = \frac{1}{\pi} \int_{0}^{\infty} dk \, \frac{\xi_{k}^{2}}{(\xi_{k}^{2} + \Delta^{2})^{3/2}} \approx \frac{1}{\pi} J_{1} - \frac{3\Delta^{2}}{\pi} J_{3},$$

$$t = \frac{1}{\pi} \int_{0}^{\infty} dk \, \frac{\xi_{k}}{(\xi_{k}^{2} + \Delta^{2})^{3/2}} \approx \frac{1}{\pi} J_{2} - \frac{3\Delta^{2}}{2\pi} J_{4},$$

$$\overline{w} = \frac{1}{\pi m} \int_{0}^{\infty} dk \, \frac{\xi_{k}}{(\xi_{k}^{2} + \Delta^{2})^{3/2}} \approx \frac{1}{\pi m} J_{2} - \frac{3\Delta^{2}}{2\pi m} J_{4},$$

$$(A2)$$

$$x = \frac{1}{\pi} \int_{0}^{\infty} dk \, \frac{1}{(\xi_{k}^{2} + \Delta^{2})^{3/2}} \approx \frac{1}{\pi} J_{3} - \frac{3\Delta^{2}}{2\pi} J_{5},$$

$$y = \frac{1}{\pi m^{2}} \int_{0}^{\infty} dk \, \frac{k^{2}}{(\xi_{k}^{2} + \Delta^{2})^{3/2}} \approx \frac{1}{\pi m^{2}} J_{32} - \frac{3\Delta^{2}}{2\pi m^{2}} J_{52},$$

$$z = \frac{\Delta^{2}}{\pi m^{2}} \int_{0}^{\infty} dk \, \frac{k^{2}}{(\xi_{k}^{2} + \Delta^{2})^{5/2}} \approx \frac{\Delta^{2}}{\pi m^{2}} J_{52}.$$

- ¹M. Gaudin, Phys. Lett. B **24**, 55 (1967).
- ²R. M. Quick, C. Esebagg, and M. de Llano, Phys. Rev. B **47**, 11 512 (1993).
- ³A. J. Leggett, J. Phys. (Paris) Colloq. **41**, C7-19 (1980).
- ⁴P. Nozières and S. Schmitt-Rink, J. Low Temp. Phys. **59**, 195 (1985).
- ⁵P. F. Williams and A. N. Bloch, Phys. Rev. B **10**, 1097 (1974).
- ⁶S. Brenner and H. Haug, Z. Phys. B **84**, 81 (1991).
- ⁷W. I. Friesen and B. Bergersen, J. Phys. **13**, 6627 (1980).
- ⁸ Chemistry and Physics of One-Dimensional Metals, Vol. 25 of NATO Advanced Study Institute, Series B: Physics, edited by I. Keller (Plenum, New York, 1977).
- ⁹R. E. Peierls, *Quantum Theory of Solids* (Oxford University Press, New York, 1955).
- ¹⁰P. W. Anderson, Phys. Rev. **112**, 1901 (1958).
- ¹¹G. Rickayzen, Phys. Rev. **115**, 795 (1959).
- ¹² A. Bardasis and J. R. Schrieffer, Phys. Rev. **121**, 1050 (1961).
- ¹³J. O. Sofo, C. A. Balseiro, and H. E. Castillo, Phys. Rev. B 45, 9860 (1992).
- ¹⁴T. Kostyrko and R. Micnas, Phys. Rev. B **46**, 1025 (1992).
- ¹⁵ A. S. Alexandrov and S. G. Rubin, Phys. Rev. B **47**, 5141 (1993).
- ¹⁶L. Belkhir and M. Randeria, Phys. Rev. B **49**, 6829 (1994).
- ¹⁷R. Micnas, J. Ranninger, and S. Robaszkiewicz, Rev. Mod. Phys. 62, 113 (1990).

- ¹⁸P. Nozières and C. Comte, J. Phys. (Paris) **43**, 1083 (1982).
- ¹⁹R. Cote and A. Griffin, Phys. Rev. B **37**, 4539 (1988): **48**, 10 404 (1993).
- ²⁰G. Fano, Nuovo Cimento **6**, 959 (1960).
- ²¹D. H. Kobe and W. B. Cheston, Ann. Phys. (N.Y.) **20**, 279 (1962).
- ²²P. Ring and P. Schuck, *The Nuclear Many-Body Problem* (Springer, Berlin, 1980).
- ²³ J. Dukelsky and P. Schuck, Nucl. Phys. A **512**, 466 (1990).
- ²⁴P. Schuck and S. Ethofer, Nucl. Phys. A **212**, 269 (1973).
- ²⁵J. Dukelsky and P. Schuck (unpublished).
- ²⁶J. Lindhard, Kgl. Danske Videnskab. Selskab. Mat. Fys. Medd. 28. No. 8 (1954).
- ²⁷L. Balents and M. Kardar, Phys. Rev. B **46**, 16 031 (1992).
- ²⁸N. N. Bogoliubov, J. Phys. (Moscow) **11**, 23 (1947).
- ²⁹ A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw-Hill, New York, 1971).
- ³⁰R. Haussmann, Z. Phys. B **91**, 291 (1993).
- ³¹Y. A. Bychkov, L. P. Gorkov, and I. E. Dzyaloshinski, Zh. Eksp. Tech. Fiz. **50**, 738 (1966) [Sov. Phys. JETP **23**, 489 (1966)].
- ³²G. Röpke, Ann. Phys. (Leipzig) **3**, 145 (1994).
- ³³P. Krüger and P. Schuck, Europhys. Lett. **27**, 395 (1994).