Quantum Condensates in Nuclear Matter: Problems

G. Röpke, D. Zablocki

Inst. Physik, Universität Rostock, Rostock, Germany

Abstract

In connection with the contribution “Quantum Condensates in Nuclear Matter” some problems are given to become more familiar with the techniques of many-particle physics.

1 Bogoliubov transformation for superfluid state

The entropy operator $S$, which is related to the (grand canonical) statistical operator via $\rho = \exp[-S/k_B]$, has in second quantization the form

$$S = S_0 + S_1 + S_2 \ldots$$

where $S_0$ is a normalization constant, the single-particle contribution has the general form

$$S_1 = \sum_{ij} s(i,j) a_i^\dagger a_j + \sum_{ij} d(i,j) a_i a_j + \sum_{ij} d^*(i,j) a_i^\dagger a_j^\dagger$$

where the Lagrange multipliers $s(i,j), d(i,j), d^*(i,j)$ are determined by the given averages when maximizing the entropy, the two-particle contribution and higher terms are neglected in the mean-field approximation considered here. Assuming that $S_1$ is hermitean and that the normal term $s(i,j)$ is diagonalized, we have

$$S_1 = \sum_p s(p) a_p^\dagger a_p + \sum_p d(p,\bar{p}) a_p a_{\bar{p}} + \sum_p d^*(p) a_p^\dagger a_p^\dagger$$

if we furthermore assume that the condensate is formed with a given spin and momentum state for the two-particle system ($p$ denotes momentum and spin quantum number). In particular we can take $s(p) = p^2/2m_\sigma - \mu_\sigma$, and the pair amplitude couples $p = p, \sigma$ with the state $\bar{p} = -p, -\sigma$.

Problem 1:

Find the transformation which diagonalizes $S_1$.

Solution:

The Bogoliubov transformation for the creation and annihilation operators reads

$$a_p = u_p b_p - v_p b_p^\dagger , \quad a_p^\dagger = u_p^* b_p^\dagger - v_p^* b_p , \quad (1)$$

$$a_p = u_p b_p + v_p b_p^\dagger , \quad a_p^\dagger = u_p^* b_p^\dagger + v_p^* b_p , \quad (2)$$

where the new operators obey the anticommutator relations

$$\{b_p, b_{p'}^\dagger\} = \delta_{p,p'}, \quad \{b_p, b_{p'}\} = \{b_{p'}^\dagger, b_p^\dagger\} = 0 \quad (3)$$
In order to get a canonical transformation, i.e. the anticommutator remains unchanged, we have to claim \( \{ a_p, a^\dagger_{p'} \} = \delta_{p,p'} \).

\[
\{ a_p, a^\dagger_{p'} \} = u_p b_p u^*_p a^\dagger_{p'} b^\dagger_{p'} - u_p b_p v^*_p b_p - v_p b^\dagger_p v^*_p b^\dagger_{p'} + v_p b^\dagger_p v^*_p b^\dagger_{p'} + u_p b^\dagger_p b_p v_p b^\dagger_{p'} - u^*_p b^\dagger_p v_p b^\dagger_{p'} + v^*_p b^\dagger_p v_p b^\dagger_{p'} + v^*_p b^\dagger_p v_p b^\dagger_{p'} + v^*_p b^\dagger_p v_p b^\dagger_{p'} + v^*_p b^\dagger_p v_p b^\dagger_{p'} + v^*_p b^\dagger_p v_p b^\dagger_{p'} + v^*_p b^\dagger_p v_p b^\dagger_{p'} \]
\[
= ([u_p]^2 + [v_p]^2) \delta_{p,p'}
\]

So it follows

\[
|u_p|^2 + |v_p|^2 = 1 . \tag{4}
\]

We now list the prefactors in \( S_1 \) where we make use of the anticommutator relations \( [a^\dagger_p, a_{p'}] = \delta_{p,p'} \). In order to achieve a diagonal transformation the inner columns of Table 1 have to vanish, i.e. after substituting \( s(t) = \epsilon_p \) and \( d(p) = \Delta_p \) we have

\[
-2 \epsilon_p (u^*_p v^*_p + u^*_p v_p) + \Delta_p (u^2_p - v^2_p) + \Delta_p (u^*_{p'} v^*_{p'} - v^2_{p'}) = 0 \tag{5}
\]

One can easily check that

\[
u_p = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 + \frac{\epsilon_p}{\sqrt{\epsilon^2_p + \Delta^2_p}} \end{pmatrix}, \tag{6} \]

\[
v_p = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 - \frac{\epsilon_p}{\sqrt{\epsilon^2_p + \Delta^2_p}} \end{pmatrix} \tag{7}
\]

solve the equations (4) and (5) with \( \epsilon_p, \Delta_p \) being real functions. Furthermore we obtain

\[
S_1(p) = \sqrt{\epsilon^2_p + \Delta^2_p} \left( b^\dagger_p b_p + b^\dagger_{p'} b_{p'} - 1 \right),
\]

which is now diagonalized.

## 2 Transition from BCS to BEC

### Problem 2:

Give the form of the wave function for the two-particle wave function including Pauli blocking for the Yamaguchi interaction (isospin singlet) at \( E = 2 \mu \). How changes the wave function in coordinate-space representation if we cross over from low densities (deuteron) to high densities (Cooper pairs)?

2
Solution:

The Schrödinger equation for the two-particle problem including Pauli blocking reads

\[ [E(1) + E(2) - E_{np}] \psi_{np}(12) + \sum_{1'2'} [1 - f(1') - f(2')] V(12, 1'2') \psi_{np}(1'2') = 0, \tag{8} \]

where \( E(1) = E(p_1) = \frac{p_1^2}{2m_1} \) denotes the kinetic energy of the single-particle state \( \{1\} = \{p_1, \sigma_1, \tau_1\} \) abbreviating linear momentum, spin and isospin, respectively. The Fermi distribution function \( f(1) = \frac{\exp\left(\frac{E(p_1) - \mu_1}{T}\right) + 1}{\exp\left(\frac{E(p_1) - \mu_1}{T}\right) + 1} \) is characterized by the temperature \( T \) and the chemical potential \( \mu_1 \).

The Yamaguchi potential is

\[ \begin{align*}
V(12, 1'2') &= -\frac{\lambda}{M} W((p_1 - p_2)/2)W((p_{1'} - p_{2'}/2))\delta_{p_1+p_2, p_{1'}+p_{2'}} \end{align*} \]

with the formfactor \( W(p) = (p^2 + \gamma^2)^{-1} \), the effective range \( \gamma = 285.8484 \) MeV and the effective coupling constant \( \lambda_{S=1, T=0} = 0.4144 \) fm\(^{-3}\) for the spin triplet, isospin singlet channel and \( M \) is taken as the average nucleon mass.

After restriction to a two-nucleon system at rest in an isospin symmetric medium \( (\mu_1 = \mu_2 = \mu; \ m_1 = m_2 = m) \), the wave function satisfying the Schrödinger equation (8) reads

\[ \psi_{\sigma}(p) = c_{\sigma}(T, \mu) \frac{W(p)}{p^2/m - \bar{E}_\sigma(T, \mu)} \tag{9} \]

with the normalization factor \( c_{\sigma}(T, \mu) \). Inserting (9) into (8) one obtains the implicit equation for the binding energy \( E_\sigma(T, \mu) \)

\[ 1 = \frac{\lambda_{S=1}^2}{m} \sum_{p'} \frac{W^2(p') [1 - 2f(p')]}{p'^2/m - \bar{E}_\sigma(T, \mu)}. \tag{10} \]

It is evident that the Pauli blocking factor in the kernel of (10) generates the \( T- \) and \( \mu- \) dependence of the binding energy.

The wave function in coordinate space is obtained by Fourier transformation,

\[ \psi_{\sigma}(r) = \frac{1}{2\pi^2 r} \int_0^\infty dp \ p \ \psi_{\sigma}(p) \sin(p \ r), \tag{11} \]

with the final result

\[ \psi_{\sigma}(r) = \frac{c_{\sigma} m}{4\pi} \frac{e^{-\sqrt{m E_{\sigma}} r} - e^{-\gamma r}}{(\gamma^2 + m E_{\sigma}) r}. \tag{12} \]

A zero binding energy defines the transition from a bound state to a scattering state (Cooper pair). The corresponding transition from negative to positive energy eigenvalues entails a character change in the wave function to oscillatory behaviour.
The Schrödinger equation for the scattering problem (with the same restrictions as above) reads \[1\]

\[(k^2 - p^2 + i\epsilon)\psi(p) = -\lambda W(p) \sum_{p'} [1 - 2f(p')]W(p')\psi(p'), \quad (13)\]

with the solution

\[
\psi(p) = \delta(p - k) - \frac{k^2 + \gamma^2}{2\pi^2} \cdot F_\sigma(k) \cdot \frac{1}{\gamma^2 + p^2} \cdot \frac{1}{k^2 - p^2 + i\epsilon} \cdot (14)
\]

where $F_\sigma(k)$ is the scattering amplitude and can be obtained by inserting \(14\) into \(13\). When we neglect Pauli-Blocking, $F_\sigma(k)$ takes the form

\[
F_\sigma(k) = \left(-ik + \left(-\gamma + \frac{\gamma^2 + k^2}{2\gamma} + \frac{(\gamma^2 + k^2)^2}{2\pi^2 \lambda_\sigma}\right)^{-1}\right). \quad (15)
\]

Including Pauli-Blocking, the numerical solution is given in \[2\]. Equivalently, one can represent the solution in terms of the phase shift $\delta_\sigma(\mu, T)$, given by

\[
F_\sigma(k) = \frac{e^{i\delta_\sigma} \sin \delta_\sigma}{k} = \frac{1}{-ik + k \cot \delta_\sigma}. \quad (16)
\]

Using \(16\) and $E = k^2/m$, one obtains the explicit form for the scattering phase shift $\delta_\sigma(E)$ from

\[
\cot \delta_\sigma(E) = -\frac{1}{2\sqrt{x}} \left(1 - x - y(1 + x)^2\right) \quad (17)
\]

where we have introduced dimensionless variables $y = \gamma^3/(\pi^2 \lambda_\sigma)$ and $x = E_\sigma/E_0$ with $E_0 = \gamma^2/m$.

In order to discuss qualitatively the Mott-Effect of vanishing bound states we consider \[3\] without Pauli-Blocking but with variable potential strength. According to the Levinson theorem, at the critical coupling strength for the dissolution of the bound state, the scattering phase shift has to jump by $\pi$ at the threshold. This critical coupling strength can be calculated by solving \(10\) or \(17\) respectively.

Let us consider the case when $E$ tends to zero ($x \to 0$). \(17\) gives

\[
\lim_{x \to 0} \cot \delta_\sigma = \frac{1}{2\sqrt{x}} \left(1 - y \right) \mid_{x \to 0} \quad (18)
\]

Using \(10\) and setting the binding energy to zero, we obtain the critical coupling $\lambda_c = \gamma^3/\pi^2$ which corresponds to $y_c = 1$. When approaching this critical coupling from both sides, we get

\[
\lim_{\lambda \to \lambda_c \pm 0} \cot \delta_\sigma(E) = \pm \infty \quad (19)
\]

which corresponds to a jump of the scattering phase shift from $\pi$ to 0, in accordance with the Levinson theorem (illustrated in Figure \[1\]).

We now want to consider the Pauli-Blocking energy shift by the example of the Deuteron.
Figure 1: The scattering phase shift as a function of energy for several values of the coupling. \( \lambda_C \) is defined in the text.

3 Pauli blocking for Gaussian bound states

Problem 3:

Construct a wave function for the bound states of 2, 3, 4 nucleons by minimizing the energy (Yamaguchi interaction) with respect to Gaussian wave functions! Calculate the Pauli blocking energy shift within first order perturbation theory! What is its dependence on temperature?

Solution:

The four-particle Schrödinger equation reads

\[
E_{nP}\psi_{nP}(1234) = [E(1) + E(2) + E(3) + E(4)] \psi_{nP}(1234) \\
+ \sum_{1'2'3'4'} \left\{ [1 - f(1) - f(2)]V(121'2')\delta_{33'}\delta_{44'} \\
+ [1 - f(1) - f(3)]V(131'3')\delta_{22'}\delta_{44'} \\
+ \text{permutations} \right\} \psi_{nP}(1'2'3'4' ).
\]
3.1 \( \alpha \)-like clusters

We make a Gaussian ansatz for the wave function, i.e.

\[
\psi(r_1, r_2, r_3, r_4) = N \chi(R)e^{-\frac{1}{\alpha^2}(r_1-R)^2+(r_2-R)^2+(r_3-R)^2+(r_4-R)^2)}, \tag{20}
\]

where \( R = (r_1 + r_2 + r_3 + r_4)/4 \), or in Jacobi-coordinates

\[
\psi(\xi_1, \xi_2, \xi_3, R) = N \chi(R)e^{-\frac{1}{\alpha^2}(\xi_1^2 + \xi_2^2 + \xi_3^2)}, \tag{21}
\]

where we have used the transformation rules

\[
R_k = \frac{1}{k} \sum_{i=1}^{k} r_i, \quad \sum_{i=1}^{n} (r_i - R_n)^2 = \frac{n-1}{i + 1} \xi_i^2. \tag{22}
\]

The Fourier transformation of the wave function reads

\[
\psi(k_1, k_2, k_3, k_4) = \int \psi(\xi_1, \xi_2, \xi_3, R)e^{-i(\xi_1 q_1 + \xi_2 q_2 + \xi_3 q_3 + KR)}d^3 \xi_1 d^3 \xi_2 d^3 \xi_3 d^3 R
\]

\[
= N \chi(K)e^{-\frac{1}{\alpha^2}(\frac{2}{3} q_1^2 + \frac{2}{3} q_2^2 + \frac{2}{3} q_3^2)} \delta_{K,k_1+k_2+k_3+k_4} \tag{23}
\]

where \( K = k_1 + k_2 + k_3 + k_4 \) and \( q_i \) are the conjugate momenta to \( \xi_i \).

3.2 Normalization

The normalization factor can be determined as usual by calculating the expectation value of the square of the wave function:

\[
\frac{1}{N^2} = \left[ \frac{\Omega_0}{(2\pi)^3} \right]^3 \int e^{-\frac{1}{\alpha^2}(\frac{2}{3} q_1^2 + \frac{2}{3} q_2^2 + \frac{2}{3} q_3^2)} d^3 q_1 d^3 q_2 d^3 q_3
\]

\[
= \left[ \frac{\Omega_0}{(2\pi)^3} \right]^3 \int e^{-\frac{1}{\alpha^2}(\frac{2}{3} q_1^2 + \frac{2}{3} q_2^2 + \frac{2}{3} q_3^2)} d^3 q_1 d^3 q_2 d^3 q_3 \right]^3
\]

\[
= \left[ \frac{\Omega_0}{(2\pi)^3} \right]^3 \frac{2}{\alpha^2} \sqrt{\frac{1}{2!}} \sqrt{\frac{3}{2!}} \sqrt{\frac{4}{2!}} \left[ \int_{-\infty}^{\infty} e^{-x^2} dx \right]^3
\]

\[
= \left[ \frac{\Omega_0}{(2\pi)^3} \right]^3 \frac{\sqrt{2}}{\alpha^3} \sqrt{\frac{\alpha^3}{\sqrt{\pi}}}
\]

so it results

\[
N^2 = N_0^2 = \left[ \frac{(2\pi)^3}{\Omega_0} \right]^3 \frac{\alpha^3}{\sqrt{2} \sqrt{\pi}}. \tag{24}
\]

3.3 Kinetic energy term

\[
\langle E_{\text{kin}} \rangle = N^2 \sum_{k_1, k_2, k_3, k_4} \frac{1}{2m} \left( k_1^2 + k_2^2 + k_3^2 + k_4^2 \right) | \psi(k_1, k_2, k_3, k_4) |^2
\]
\[
\begin{align*}
\sum_K & \frac{1}{8m} |\chi(K)|^2 K^2 \\
+ N^2 \sum_{q_1 q_2} \frac{1}{2m} \left( \frac{2}{3} q_1^2 + \frac{4}{3} q_2^2 \right) e^{-\alpha^2 (\frac{2}{3} q_1^2 + \frac{2}{3} q_2^2 + \frac{2}{3} q_3^2)} \\
= & \ E_{\text{kin}}^K + N^2 \sum_{q_1 q_2} \frac{1}{2m} \frac{\partial}{\partial (\frac{1}{2} \alpha^2)} e^{-\frac{\alpha^2}{2} (\frac{2}{3} q_1^2 + \frac{2}{3} q_2^2 + \frac{2}{3} q_3^2)} \\
= & \ E_{\text{kin}}^K + N^2 \frac{1}{2m} \frac{1}{\alpha} \frac{\partial}{\partial \alpha} N^2 \\
= & \ E_{\text{kin}}^K + \frac{1}{2m} \frac{9}{\alpha^2}
\end{align*}
\]
where we explicitly separated the motion of the total momentum \( K \).

### 3.4 Potential energy term

For a separable potential we can calculate the potential part of the energy as

\[
\langle E_{\text{pot}} \rangle = -\frac{3\lambda_s + \lambda_t}{\Omega_0} \sum_{q_1 q_2 q_3} w(q_1) w(q_1') \psi(q_1, q_2, q_3, K) \psi(q_1', q_2, q_3, K) \\
= -\frac{3\lambda_s + \lambda_t}{\Omega_0} \sum_{q_1 q_2 q_3 K, q_1'} w(q_1) w(q_1') N^2 |\chi(K)|^2 \\
\times e^{-\frac{\alpha^2}{2} (\frac{2}{3} q_1^2 + \frac{2}{3} q_2^2 + \frac{2}{3} q_3^2)} e^{-\frac{\alpha^2}{2} (\frac{2}{3} q_1'^2 + \frac{2}{3} q_2'^2 + \frac{2}{3} q_3'^2)} \\
= -\frac{3\lambda_s + \lambda_t}{\Omega_0} \frac{1}{e^{-\frac{\alpha^2}{2} 2q^2}} \sum_{q, q'} w(q) w(q') e^{-\frac{\alpha^2}{2} (q^2 + q'^2)} \\
= -\frac{3\lambda_s + \lambda_t}{\Omega_0} \frac{1}{e^{-\frac{\alpha^2}{2} 2q^2}} \left[ \sum_{q} w(q) e^{-\frac{\alpha^2}{2} q^2} \right]^2.
\]

As an example we assume the potential to be of Gaussian type \( w(q) = \exp\{-q^2/\gamma^2\} \),
this leads to

\[
\langle E_{\text{pot}} \rangle = -\frac{3\lambda_s + \lambda_t}{(2\pi)^3} \frac{1}{e^{-\frac{\alpha^2}{2} 2q^2}} \left[ \int e^{-\frac{\alpha^2}{2} q^2} e^{-\frac{\alpha^2}{2} q^2} d^3q \right]^2 \\
= -24\frac{\lambda_s + \lambda_t}{(2\pi)^3} \frac{\alpha^3 \sqrt{\pi}}{\left( \frac{2}{\gamma^2} + \alpha^2 \right)^2}.
\]

So finally the total energy is given by

\[
\langle H_{\text{int}} \rangle = \langle H \rangle - E_{\text{kin}}^K = \frac{9}{2} \frac{1}{ma^2} - 24\frac{\lambda_s + \lambda_t}{(2\pi)^3} \frac{\alpha^3 \sqrt{\pi}}{\left( \frac{2}{\gamma^2} + \alpha^2 \right)^2}.
\] (25)
3.5 Model calculation

We can now minimize this expression with respect to the variational parameter $\alpha$ and fit the binding energy for the $\alpha$ particle by adjusting our model parameters. We obtain

$$\lambda_t = 1317.8 \text{ MeV fm}^{-3}, \quad \lambda_s = 667 \text{ MeV fm}^{-3}$$

and therefore

$$\alpha = 8.288 \cdot 10^{-3} \text{ MeV}^{-2},$$

which gives us a binding energy of the $\alpha$ particle of $-28.2$ MeV.

For the other bound states with less nucleons, this works in a similar way.

3.6 Pauli blocking shift

Now we want to calculate the Pauli blocking shift due to finite temperature. We will consider a bound state of 2 nucleons. For 3 and 4 nucleons this works similar but is more cumbersome. From Eq. (10) we know that the exact wave function in the vacuum satisfies

$$1 = \frac{\lambda_s m}{\int |\psi(p')|^2 p'^2 dp'}$$

In perturbation theory we expand the binding energy around its vacuum value, i.e. $|E_\sigma| = E^0_\sigma - \Delta E^{\text{Pauli}}(T, \mu)$ where the minus sign is because the binding energy is negative ($E_\sigma = -|E_\sigma|$).

$$1 = \frac{\lambda_s m}{\int |\psi(p')|^2 p'^2 dp'} \frac{W^2(p')}{p'^2/m + E^0_\sigma - \Delta E^{\text{Pauli}}(T, \mu)}$$

$$= \frac{\lambda_s m}{\int |\psi(p')|^2 p'^2 dp'} \frac{W^2(p')}{p'^2/m + E^0_\sigma - \Delta E^{\text{Pauli}}(T, \mu)}$$

$$= \frac{\lambda_s m}{\int |\psi(p')|^2 p'^2 dp'} \left( 1 - 2f(p') + (1 - 2f(p')) \frac{\Delta E^{\text{Pauli}}(T, \mu)}{p'^2/m + E^0_\sigma} + \mathcal{O}((\Delta E^{\text{Pauli}})^2) \right)$$

Dropping higher order terms we arrive at

$$\Delta E^{\text{Pauli}}(T, \mu) = \frac{\int |\psi(p)|^2 (p^2/m + E^0_\sigma)^2 f(p)^2 dp}{\int |\psi(p)|^2 p^2 dp},$$

we have assumed $2f(p')$ to be small against 1 and used the expression for the wave function $\psi(p)$ given in Eq. (11).

References

[1] Yamaguchi, Y. // Phys. Rev. 1954. V.95.P.1628.
[2] Schmidt, M., Röpke, G. // phys. stat. sol. (b). 1987. V.139.P.441.