PARTICLE-HOLE STRUCTURE OF FINITE SYSTEMS WITH PAIRING

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In order to ascertain how many particle and hole pairs appear in finite superconducting or superfluid systems at various particle numbers N and pairing strengths g in the BCS Hamiltonian (H_{BCS}) the eigenfunctions of H_{BCS} with a fixed N are constructed as superposition of two particle–two hole excitations. For an even system with $(\Omega_p + \Omega_h)$ two-fold degenerate levels among wich Ω_h levels are occupied at $g = 0$ and Ω_p ones are vacant $(N = 2\Omega_h)$ such functions e.g. for zero seniority can be written in the form

$$|\Psi\rangle = \beta_0 \left\{ 1 + \sum_{n\geq 1, s, t} \beta_{st}(n) B_s^+(n) \tilde{B}_t^+(n) \right\} |\tilde{0}\rangle, \tag{1}$$

$|\tilde{0}\rangle$ is the Hartree—Fock vacuum, $B_s^+(n) = \sum_{\mu_1 \ldots \mu_n} \alpha(\mu_1 \ldots \mu_n) p_{\mu_1}^+ p_{\mu_2}^+ \cdot \ldots \cdot p_{\mu_n}^+$, $p_\mu^+ = a_\mu^+ a_{\bar{\mu}}^+$, a_μ^+ is a particle creation operator in state μ, $\bar{\mu}$ is a time conjugated state. $\tilde{B}_t^+(n)$ is analogous with $B_t^+(n)$ but is composed of hole creation operators $\tilde{p}_\nu^+ = \tilde{a}_\nu^+ \tilde{a}_{\bar{\nu}}^+$. In the particle-hole $(p-h)$ representation H_{BCS} is divided into H_p, H_h and particle-hole interaction v:

$$\begin{gathered} H_p = \sum_{\mu=1}^{\Omega_p} (\varepsilon_\mu - \lambda) n_\mu - g P^+ P; \quad H_h = -\sum_{\nu=1}^{\Omega_h} (\varepsilon_\nu - \lambda) \tilde{n}_\nu - g \tilde{P}^+ \tilde{P}; \\ P^+ = \sum_\mu p_\mu^+; \quad \tilde{P}^+ = \sum_\nu \tilde{p}_\nu^+; \quad v = g\left(P^+ \tilde{P}^+ + \tilde{P} P\right); \end{gathered} \tag{2}$$

$$\left[H_p, B_s^+(n)\right] = E_s(n) B_s^+(n); \left[H_h, \tilde{B}_t^+(h)\right] = \tilde{E}_t(n) \tilde{B}_t^+(n). \tag{3}$$

For systems with equidistant levels at $\Omega_p = \Omega_h$ and $\lambda = (\varepsilon_F + \varepsilon_{F+1})/2$ sets of $E_s(n)$ and $E_t(n)$ coincide. Energies of zero seniority states and amplitudes $\beta_{st}(n)$ in (1) $(n \geq 1, b_{st}(0) = 1)$ are determined by the system of equations:

$$\begin{gathered} \beta_{st}(n)\left[E_s(n) + \tilde{E}_t(n) - E\right] + g \sum_{s't'} \beta_{s't'}(n+1) \langle sn | P | s'n+1 \rangle \langle tn | \tilde{P} | t'n+1 \rangle + \\ + g \sum_{s't'} \beta_{s't'}(n-1) \langle s'n-1 | P | sn \rangle \langle t'n-1 | \tilde{P} | tn \rangle = 0; \\ E = \sum [\beta_{st}(n)]^2 \left[E_s(n) + E_t(n) - E\right] + \\ + 2g \sum \beta_{st}(m) \beta_{s't'}(m+1) \langle sm | P | s'm+1 \rangle \langle tm | P | t'm+1 \rangle. \end{gathered} \tag{4}$$

Eqs. (4) include $p-h$ transfer matrix elements, e.g. $\langle sm|P|s'm+1\rangle = \langle\tilde{0}|B_s(m)PB^+_{s'}(m+1)|\tilde{0}\rangle$. Energies $E_s(n)$ and $\tilde{E}_t(n)$ standing in Eqs. (3), (4) can be calculated by means of recurrent procedure: at first for all n e.g. particle operators $B^+_s(\omega,n)$ are defined for ω levels $\left(\Omega_p > \omega \geq n, B^+_s(\omega=n,n) = p^+_1 p^+_2 \ldots p^+_n\right)$, after that operators $B^+_s(\omega+1,n)$ are expressed through $B^+_{s'}(\omega,n)$ and $B^+_{s''}(\omega,n-1)$:

$$B^+_s(\omega+1,n) = \sum_{s'} \psi_{ss'}(n) B^+_{s'}(\omega,n) + \sum_{s''} \psi_{ss''}(n-1) B^+_{s''}(\omega,n-1)\, p^+_{\omega+1}.$$

Amplitudes $\psi(n)$, $\psi(n-1)$ and eigenvalues $E_s(\omega+1,n)$ are found with the help of equations:

$$\psi_{ss'}(n)\left[E_{s'}(\omega,n) - E_s(\omega+1,n)\right] - g\sum_{s''}\psi_{ss''}(n-1)\langle n-1s''|P(\omega)|ns'\rangle = 0,$$

$$\psi_{ss''}(n-1)\left[E_{s''}(\omega,n-1) + E_{\omega+1} - E_s(\omega+1,n)\right] - g\sum_{s'}\psi_{ss'}(n)\langle n-1s''|P(\omega)|ns'\rangle = 0.$$

Thus, several additional diagonalizations are required to solve Eqs. (4). However, at high enough particle numbers (that occures in deformed nuclei and nano-clusters) and at realistic values of g transfer matrix elements between states $|s_0 n\rangle$ and $|s'_0 n+1\rangle$, where s_0, s'_0 correspond to states with minimal energies at given n and $n+1$, considerably exceed those between other states [1]. This paves the way to obtain approximate solutions with smaller amount of diagonalization.

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1. A.K.Vlasnikov, A.V.Lunev, V.M.Mikhajlov // Bull. Russ. Acad. Sci. Phys. 2013. V.77. P.880.