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 $(H_{\rm BCS})$ the eigenfunctions of $H_{\rm BCS}$ 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

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

$|\tilde{0}\rangle$ 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 $H_{\rm BCS}$ is divided into H_p, H_h and particle-hole interaction v:

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

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

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:

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

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.