Thermal and Quantal Fluctuations for Fixed Particle Number in Finite Superfluid Systems

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We investigate fluctuations and even-odd effects in small superfluid systems at finite temperature by means of the static path approximation (SPA) plus random-phase approximation (RPA) treatment, where exact number parity projection is introduced. The RPA correction to the SPA is evaluated exactly. Results are given first for a schematic 20-level pairing model, where an excellent agreement with the exact canonical results is obtained both for even and odd systems, and then for a heavy nucleus, where the smoothing of the BCS transition and the even-odd effects in the pairing energy and specific heat are examined. [S0031-9007(98)05372-1]

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Fluctuations play an important role in small quantum systems like finite nuclei. Statistical fluctuations in the order parameters smooth out the sharp phase transitions arising at finite temperature in the mean field approximation [1,2], and can be microscopically described by means of the static path approximation (SPA) [2–5]. At the same time, the constraint of a fixed particle number may imply significant deviations from normal grand canonical (GC) statistics, leading, for instance, to even-odd effects in small superfluid systems, well known at zero temperature [6]. The detailed thermal behavior of even-odd effects is, however, less known. These subjects have recently attracted renewed interest also in solid state physics due to the development of ultrasmall superconducting metallic grains [7], where fluctuations and even-odd effects become also relevant [8]. These were examined at finite temperature with number parity projected BCS [8–10], which, however, still exhibits a sharp transition and is thus no longer accurate near T_c.

The aim of this Letter is to present a fully microscopic and general treatment of fluctuations *and* even-odd differences in finite superfluid systems, by means of the SPA + RPA (random-phase aproximation) approach [11–14], to be denoted as correlated SPA (CSPA), where we introduce exact number parity (NP) projection [10]. The CSPA incorporates small amplitude quantal fluctuations to the SPA and has been shown to provide a very accurate evaluation of the GC partition function (PF) in correlated systems for not too low temperatures, constituting a simple alternative to more complex approaches [15]. Here we evaluate the RPA correction to the SPA in closed form for general superfluid systems, in terms of the *extended* quasiparticle RPA energies. Results are given for a 20-level pairing model, where NP projection is shown to be essential for the agreement with the exact canonical results, and for the nuclei ^{164}Er and ^{165}Er, where even-odd effects in the pairing energy and specific heat are examined.

We consider a general two-body Hamiltonian written as $H = H_0 - \frac{1}{2}\sum_\nu v_\nu Q_\nu^2$ [15], where H_0, Q_ν are Hermitian one-body fermion operators of the general form

$$Q = \sum_{i,j}[Q_{ij}^{11}c_i^\dagger c_j + \tfrac{1}{2}(Q_{ij}^{20}c_i^\dagger c_j^\dagger + Q_{ij}^{02}c_i c_j)] = q + \tfrac{1}{2}(c^\dagger c)\mathcal{Q}\binom{c}{c^\dagger}, \quad \mathcal{Q} = \begin{pmatrix} Q^{11} & Q^{20} \\ Q^{02} & -(Q^{11})^t \end{pmatrix}, \quad (1)$$

with $q = \frac{1}{2}\sum_i Q_{ii}^{11}$. Using the Hubbard-Stratonovich transformation, the GC PF can be written as the auxiliary field path integral [4,15]

$$Z = \int D[x]\,\mathrm{Tr}\,\hat{T}\exp\left\{-\int_0^\beta H[x(\tau)]\,d\tau\right\}, \quad (2)$$

$$H(x) = H_0 - \mu N + \sum_\nu \frac{x_\nu^2}{2v_\nu} - x_\nu Q_\nu = E_0(x) + \tfrac{1}{2}(c^\dagger c)\mathcal{H}(x)\binom{c}{c^\dagger},$$

where $\hat{T}$ denotes time ordering. Using now a Fourier expansion $x_\nu(\tau) = \sum_n x_{\nu n}e^{i\omega_n\tau}$, with $\omega_n = 2\pi n/\beta$ and $D[x] = \prod_{\nu,n}(\beta/2\pi v_\nu)^{1/2}dx_{\nu n}$, the CSPA is obtained retaining the full integration over the *static* variables $x_{\nu 0}$, to include large amplitude static fluctuations, and integrating over $x_{\nu n\neq 0}$ in the saddle point approximation for every $x_{\nu 0}$. The final result is [13,14]

$$Z_{\text{CSPA}} = \int_{-\infty}^{\infty} d(x)\,\mathrm{Tr}\exp[-\beta H(x)]C_{\text{RPA}}(x), \quad (3)$$

$$C_{\text{RPA}}(x) = \prod_{n=1}^{\infty}\mathrm{Det}[\tilde{A}_{\nu\nu'}^{-1}(i\omega_n)] = \prod_{\alpha>0}\frac{\omega_\alpha\sinh[\frac{1}{2}\beta\lambda_\alpha]}{\lambda_\alpha\sinh[\frac{1}{2}\beta\omega_\alpha]}, \quad (4)$$

$$\tilde{A}_{\nu\nu'}(\omega) = \delta_{\nu\nu'} - \tfrac{1}{2}v_\nu\sum_\alpha \mathcal{Q}_{\nu\alpha}^*\frac{f_\alpha}{\lambda_\alpha - \omega}\mathcal{Q}_{\nu'\alpha}, \quad (5)$$

where $d(x) = \prod_\nu(\beta/2\pi v_\nu)^{1/2}dx_\nu$ and ω_α are the thermal quasiparticle RPA energies defined as the eigenvalues of

$$A_{\alpha\alpha'} = \lambda_\alpha\delta_{\alpha\alpha'} - \tfrac{1}{2}f_\alpha\sum_\nu v_\nu\mathcal{Q}_{\nu\alpha}\mathcal{Q}_{\nu\alpha'}^*. \quad (6)$$

Here we used the diagonal quasiparticle basis where $\mathcal{H}_{kk'}(x) = \lambda_k \delta_{kk'}$, with $\lambda_\alpha \equiv \lambda_{k'} - \lambda_k$, $f_\alpha \equiv f_k - f_{k'}$, $f_k = (1 + e^{\beta\lambda_k})^{-1}$ Fermi probabilities and $\mathcal{Q}_{\nu\alpha} \equiv (\mathcal{Q}_\nu)_{kk'}$ the elements of the extended matrices (1) in this basis. The label α comprises *all* pairs $k \neq k'$ of the matrices (1) (including both signs of λ_k) and the product in (4) runs over all pairs $k < k'$, i.e., all ω_α of a definite sign. As

$$\mathrm{Det}[\tilde{A}_{\nu\nu'}(\omega)] = \mathrm{Det}[A_{\alpha\alpha'} - \omega\delta_{\alpha\alpha'}]/\mathrm{Det}[(\lambda_\alpha - \omega)\delta_{\alpha\alpha'}],$$

the nontrivial energies $\omega_\alpha \neq \lambda_\alpha$ fulfill $\mathrm{Det}[\tilde{A}_{\nu\nu'}(\omega)] = 0$.

The integrand in (3) represents a thermodynamic probability, with $\mathrm{Tr}\, e^{-\beta H(x)}$ an independent quasiparticle PF which is maximum at the fundamental self-consistent mean field $x_\nu = v_\nu \langle Q_\nu \rangle_x$, while Eq. (4) is proportional to the ratio of the PF of independent RPA bosons of energies ω_α, to that of quasiparticle pairs of energies λ_α considered as bosons [13]. Overcounting is thus avoided. The ω_α become the conventional thermal RPA energies at the self-consistent mean field. For arbitrary x, the lowest ω_α's may become imaginary (or complex) at low temperatures but $C_{\mathrm{rpa}}(x)$ remains finite and positive both for $\omega_\alpha = 0$ and for imaginary ω_α if $\beta|\omega_\alpha| < 2\pi$. This condition will be violated at very low temperatures $T < T_c^*$, where the small amplitude approximation for $x_{\nu n\neq 0}$ at unstable values of $x_{\nu 0}$ [11] will break down. For the handling of repulsive terms $v_\nu < 0$, see [13].

In the case of a pairing Hamiltonian

$$H = \sum_k \varepsilon_k (c_k^\dagger c_k + c_{\bar{k}}^\dagger c_{\bar{k}}) - g P^\dagger P, \quad P^\dagger = \sum_k c_k^\dagger c_{\bar{k}}^\dagger, \tag{7}$$

with $\bar{k}$ the time reversed states, Eq. (3) becomes

$$Z_{\mathrm{CSPA}} = \frac{2\beta}{g} \int_0^\infty \Delta d\,\Delta e^{-\beta\Delta^2/g} Z(\Delta) C_{\mathrm{RPA}}(\Delta), \tag{8}$$

$$Z(\Delta) = \mathrm{Tr}\exp[-\beta h(\Delta)] = \prod_k 4 e^{-\beta\gamma_k} \cosh^2[\tfrac{1}{2}\beta\lambda_k],$$

$$h(\Delta) = \sum_k \varepsilon_k' (c_k^\dagger c_k + c_{\bar{k}}^\dagger c_{\bar{k}}) - \Delta(P^\dagger + P) + \tfrac{1}{2} g\Omega,$$

$$C_{\mathrm{RPA}}(\Delta) = \prod_k \frac{\omega_k \sinh[\beta\lambda_k]}{2\lambda_k \sinh[\frac{1}{2}\beta\omega_k]}, \tag{9}$$

where $\lambda_k = [\varepsilon_k'^2 + \Delta^2]^{1/2}$ are the quasiparticle energies, $\varepsilon_k' = \varepsilon_k - \mu - g/2$, $\gamma_k = \varepsilon_k - \mu$, $\Omega = \sum_k 1$, and $\omega_k(\Delta)$ are the eigenvalues of the reduced RPA matrix

$$\begin{pmatrix} 2\lambda_k\delta_{kk'} - \frac{g}{2}\tilde{f}_k(u_k u_{k'} + 1) & -\frac{g}{2}\tilde{f}_k(u_k u_{k'} - 1) \\ \frac{g}{2}\tilde{f}_k(u_k u_{k'} - 1) & \frac{g}{2}\tilde{f}_k(u_k u_{k'} + 1) - 2\lambda_k\delta_{kk'} \end{pmatrix}$$

with $u_k = \varepsilon_k'/\lambda_k$, $\tilde{f}_k = \tanh[\frac{1}{2}\beta\lambda_k]$. The SPA is obtained if $C_{\mathrm{RPA}}(\Delta)$ is omitted, while the BCS PF is $e^{-\beta\Delta_0^2/g} Z(\Delta_0)$, with $\Delta_0 = g\langle P^\dagger \rangle_{\Delta_0}$ the self-consistent gap. BCS represents the limit of infinite particle number or volume. Deviations from BCS increase as the size of the system decreases, and are appreciable for $\delta > 0.01$, where $1/\delta = kT_c/\varepsilon$ is the effective size parameter [2], with ε the average single particle level spacing at the Fermi surface and T_c the BCS critical temperature. In heavy nuclei, typically $\delta \approx 0.6$.

Equation (8) provides an accurate approximation to the GC PF for $T > T_c^*$. However, in small systems with fixed particle number N, the canonical PF should be employed. Although exact number projection is difficult to implement in the CSPA when $[H(x), N] \neq 0$ [5], it is easy to apply NP projection [9,10,16] *exactly*. The CSPA can be directly applied in a restricted ensemble defined by a projector P if $[P, H(x)] = 0$ and the eigenstates of $PH(x)$ are independent quasiparticle states. We should replace the GC trace in (3) by $\mathrm{Tr}\, P e^{-\beta H(x)}$, and f_k in (6) by the projected occupation probability. The NP projector is

$$P_\sigma = \tfrac{1}{2}(1 + \sigma e^{i\pi N}), \quad \sigma = \pm 1,$$

and fulfills $[P_\sigma, H(x)] = 0$. In the diagonal basis, $H(x) = E_0 + \sum_k \lambda_k (a_k^\dagger a_k - \frac{1}{2})$, with $a_k^\dagger, a_k$ quasiparticle operators, and states with even or odd quasiparticle number have definite number parity. Thus,

$$Z_\sigma \equiv \mathrm{Tr}\, P_\sigma e^{-\beta H(x)} = \tfrac{1}{2}(Z_+ + \sigma' Z_-),$$

$$Z_\pm = e^{-\beta E_0} \prod_k e^{\frac{1}{2}\beta\lambda_k}(1 \pm e^{-\beta\lambda_k}),$$

with $\sigma' = \sigma$ $(-\sigma)$ if the quasiparticle vacuum has even (odd) number parity [6]. The NP projected probability is $f_{k\sigma} = \frac{1}{2} - \beta^{-1}\partial \ln Z_\sigma / \partial\lambda_k$. In the pairing case,

$$Z_\sigma(\Delta) = \tfrac{1}{2} Z(\Delta)\left[1 + \sigma \prod_k \tanh^2(\tfrac{1}{2}\beta\lambda_k)\right], \tag{10}$$

and $\tilde{f}_k \to \tilde{f}_{k\sigma} = \beta^{-1}\partial \ln Z_\sigma(\Delta)/\partial\lambda_k$ in the RPA matrix.

The *canonical* PF can then be obtained by performing the number projection in the saddle point approximation for each Δ [16,17], which yields

$$Z_C(\Delta) \approx 2 Z_\sigma(\Delta) e^{-\beta\mu(\Delta)N} \Big/ \sqrt{2\pi\sigma_N^2(\Delta)}, \tag{11}$$

with $\mu(\Delta)$ obtained from $\beta^{-1}\partial \ln Z_\sigma(\Delta)/\partial\mu = N$ (constraint) and $\sigma_N^2(\Delta) = \beta^{-2}\partial^2 \ln Z_\sigma(\Delta)/\partial\mu^2$ [$C_{\mathrm{RPA}}(\Delta)$ should be also included in these derivatives, but RPA corrections in N are normally negligible]. The important even-odd effects are exactly taken into account by the NP projection, while the second projection (11) removes the remaining statistical fluctuations (σ_N^2). If $\mu(\Delta)$ is nearly constant, Eq. (11) can be applied after Δ integration, with a fixed μ. In general, the present form is preferable since the variation of μ with the static variables x may be non-negligible [17]. Application of Eq. (11) without previous NP projection fails to correctly describe even-odd differences for low T (see below).

We first consider a 20-level model ($\Omega = 10$) where the full canonical PF can be calculated exactly [16]. As seen in Fig. 1 for uniform level spacing 0.2ε and $g = 0.2\varepsilon$, for which $T_c = 0.44\varepsilon$ ($\varepsilon \approx 1$ MeV for nuclear scales) NP projected CSPA leads to almost *exact* results for the canonical energy $E = -\partial \ln Z_C/\partial\beta$, and the pairing energy $g\langle P^\dagger P\rangle = (g/\beta)\partial \ln Z_C/\partial g$, *both* in the even ($N = \Omega$) and odd ($N = \Omega + 1$) cases, for $T > T_c^* \approx 0.3T_c$ (CSPA breakdown; results are plotted for $T > T_c^* + 0.02\varepsilon$). The NP projection is required for the agreement with the exact canonical results for $T < T_c$, and becomes *essential* for N odd at low T, where results without NP projection are essentially the average of those for neighboring even N (lower in energy). For low T, NP projection increases slightly the pairing energy for N even, but decreases it considerably for N odd, increasing the odd total energy [for $T \to 0$, $\Delta E_{\text{odd-even}} \approx 0.91\varepsilon$ (exact), while $\lambda_1(\Delta_0) \approx \Delta_0 \approx 0.86\varepsilon$ in BCS]. For $T > T_c$, the effects of NP projection become small, and even though the pairing energy is much larger than the BCS value, it is nearly equal in even and odd systems and does not give rise to appreciable even-odd effects.

The RPA corrections increase the pairing energy in both the even and odd cases, decreasing the total energy. Part of these corrections account for the exchange terms, missing in the SPA PF at low T. These were included in the SPA and BCS results for the pairing energy, by evaluation as expectation value [5], and reduce the difference with the CSPA result (this procedure also corrects the wrong low T behavior of the SPA energy derived from the PF [5]). The NP and RPA effects can be visualized in the effective free energy potential (Fig. 2). At low T, NP projection makes $F(\Delta)$ slightly deeper for N even, but shallower and with the minimum shifted to a smaller Δ for N odd, while $C_{\text{rpa}}(\Delta)$ decreases $F(\Delta)$ almost uniformly in both cases.

The extended RPA energies fulfill $\omega_k^2 < 4\lambda_k^2\ \forall k, \Delta$ for $g > 0$ (Fig. 2), implying $C_{\text{RPA}}(\Delta) > 1\ \forall\Delta$ for $T > T_c^*$. The lowest one ω_1 is the continuation of the Goldstone mode associated with the broken $U(1)$ symmetry [13] and *dominates* the RPA correction (4), vanishing at the superfluid BCS solution and becoming *imaginary* for $\Delta < \Delta_0$. The minimum of ω_1^2 determines the maximum of $C_{\text{rpa}}(\Delta)$ and the CSPA breakdown. For $T > T_c$, all ω_k are real $\forall\Delta$, but ω_1 still deviates considerably from the rest for large Δ, giving rise to a non-negligible RPA correction for $T < 3T_c$. The effect of NP projection on the ω_k is small, and visible mainly in ω_1, which will now vanish at the maximum of $Z_\sigma(\Delta)$. At fixed β, μ, Δ, $\tilde{f}_{k-} < \tilde{f}_{k+}$ in the RPA matrix, so that $\omega_{1-}^2 > \omega_{1+}^2$. The RPA corrections are thus slightly smaller in the odd case.

We next consider the deformed nuclei ^{164}Er and ^{165}Er with monopole pairing. We set $H_0 = H_s - \hbar\omega_0\beta_d Q_{20}$, with H_s a spherical part and Q_{20} a quadrupole operator, and use the Baranger-Kumar configuration space for the valence nucleons [18] (for neutrons, the $n = 5, 6$ major shells with 98 single particle states, the dimension of the canonical many-body space being 3.8×10^{23} for ^{164}Er), together with their parameters for H_s, ω_0, Q_{20}, and the pairing strengths. For neutrons, the BCS pairing transition occurs at $T_c \approx 0.45$ MeV. The deformed to spherical transition in the thermal HF approximation occurs at $T \approx 1.7$ MeV for a quadrupole interaction in these nuclei, so that for $T < 1$ MeV we can approximately consider β_d fixed at the $T = 0$ self-consistent value. Quadrupole

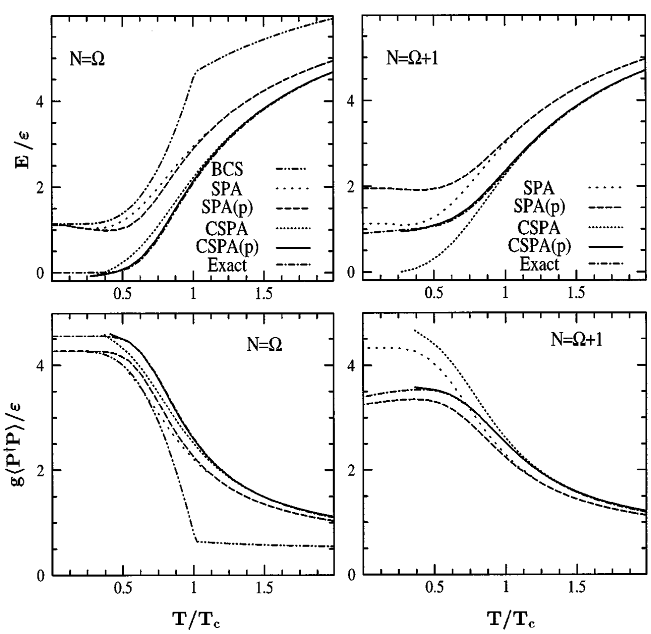

FIG. 1. Excitation energy from the even ground state (top) and pairing energy (bottom) as a function of temperature in the schematic 20-level model (see text) for $N = 10$ (left) and $N = 11$ (right) particles. SPA(p) and CSPA(p) depict the canonical number parity projected results, while SPA and CSPA those without NP projection. Standard BCS and exact canonical results [which overlap with those of CSPA(p) for $T > T_c^*$] are also depicted.

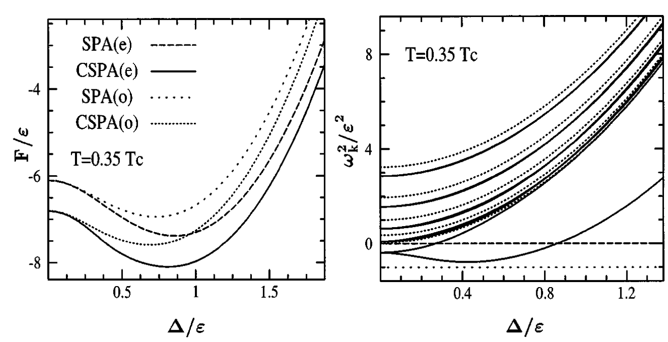

FIG. 2. The free energy $F(\Delta) = -T\ln[Z_C(\Delta)C_{\text{RPA}}(\Delta)]$ (left) as a function of Δ at fixed T, for the even (e) and odd (o) cases of Fig. 1. SPA depicts $-T\ln Z_C(\Delta)$. Right: Squared RPA energies ω_k^2 (solid lines) and quasiparticle pair energies $(2\lambda_k)^2$ (dotted lines) as a function of Δ at fixed T for the even case. The lowest RPA energy vanishes at the BCS gap $\Delta_0/\varepsilon = 0.84$. The lowest horizontal dotted line indicates the breakdown value $-(2\pi T)^2$.

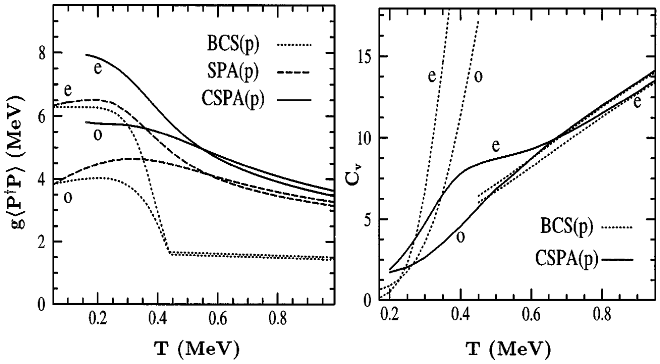

FIG. 3. The neutron pairing energy (left) and the neutron contribution to the specific heat (right), in ^{164}Er (*e*) and ^{165}Er (*o*), according to NP projected BCS, CSPA, and SPA (left).

shape fluctuations have a negligible influence for $T < 1$ MeV on the magnitudes depicted.

CSPA and SPA results for the neutron pairing energy (Fig. 3) are compared with NP projected BCS, where the self-consistent gap Δ_0 is determined from the maximum of $Z_\sigma(\Delta)$ (the BCS pairing energy is then evaluated as $g\langle P^\dagger P\rangle_{\Delta\sigma}$). NP projection decreases the BCS gap in the odd case (for $T \to 0$, $\Delta_+ = \Delta \approx 0.8$ while $\Delta_- \approx 0.54$ MeV), but the sharp transition is still present at approximately the same T_c. The transition becomes significantly washed out in the SPA and CSPA, particularly in the odd case, and deviations from BCS are considerable. This is also seen in the neutron contribution to the specific heat, $C_v = dE_n/dT$, where in the odd case no remnant of the BCS discontinuity is left in the projected CSPA result, while in the even case a smoothed kink is still visible (which is flattened in a GC treatment). Even-odd differences become nevertheless small in the CSPA for $T > 0.6$ MeV (where they are given by standard GC statistics, with vanishing effects from NP projection). The CSPA breakdown occurs at $T_c^* \approx 0.15$ MeV (at $\Delta \approx 0.4$ MeV) and the NP projected CSPA results can be considered "exact" for $T > 0.25$ MeV. The CSPA corrections increase the SPA pairing energy but practically do not affect the even-odd difference or the shape of the specific heat (which is slightly lower in the SPA) for $T > 0.25$ MeV. We also remark that for $T < 1$ MeV, the behavior of the specific heat is completely disentangled from finite configuration space effects, which lead to a Schottky-type peak at $T \approx 2.5$ MeV, well above T_c.

In conclusion, we have introduced NP projection in the CSPA and shown that its effects, together with those of thermal fluctuations, are essential for an accurate description of even-odd effects in small superfluid systems. For the same size parameter, the smoothing of the BCS transition is more pronounced in the odd system due to the smaller average pairing energy. Even-odd differences become nevertheless small for $T > T_c$. The high accuracy of the present projected CSPA treatment also suggests that it may provide a simple yet highly reliable (and elegant) alternative for describing correlated finite fermion systems at finite temperature, at least for interactions containing a few separable terms.

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