Effects of repulsive forces on thermal fluctuations

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We investigate the treatment of repulsive interactions in the presence of thermal fluctuations in hot finite systems, within the context of the static path approximation (SPA) and the ensuing SPA plus random-phase approximation treatment. We show that static repulsive variables can be correctly treated in the stationary-phase approximation. Results are shown for models containing both attractive and repulsive terms, where the accuracy of the previous methods and the effects of repulsive terms are analyzed. [S0556-2813(97)05008-5]

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I. INTRODUCTION

The description of finite nuclei at finite temperature [1] has attracted renovated interest in recent years. From the experimental side, the recent development of crystal-ball detectors will provide more detailed information of excited nuclei, particularly in the quasicontinuum region. On the theoretical side, there has been a noteworthy improvement in the microscopic treatment of nuclei at finite temperature, through the application of the Hubbard-Stratonovich (HS) transformation [2] and the ensuing path-integral representation of the partition function. Using Monte Carlo techniques, these path integrals can in principle be calculated exactly in finite configuration spaces [3].

At the same time, the path-integral formulation allows one to derive a very elegant microscopic theory of statistical fluctuations through the static path approximation (SPA) [4–9], which contains the most significant finite-size effects beyond mean field at finite temperature, such as the coexistence of shapes in transitional regions and the concomitant smoothing of the sharp mean-field phase transitions. These fluctuations can also be qualitatively introduced by means of semimacroscopic Landau prescriptions [10–12] (which, however, do not yield a microscopic partition function like the SPA) and have been shown to be essential for the description of the basic features of giant dipole resonances [13,14] and of collective transitions in the decay of hot nuclei [15]. Further correlations beyond SPA can be incorporated with the SPA plus random-phase approximation (RPA) treatment [16–20], which includes in addition the small-amplitude quantal fluctuations and was shown to be very accurate for *attractive* interactions, above a certain breakdown temperature, normally very small.

The SPA and SPA plus RPA [to be denoted for brevity as correlated SPA (CSPA)] have so far been applied to pure attractive forces. The aim of this work is to analyze the extension of these methods to Hamiltonians that also contain *repulsive* terms. This is important for the microscopic understanding of the pairing plus quadrupole plus dipole Hamiltonian, a minimal microscopic model for the description of giant resonances in hot nuclei [21,22], where the dipole term is repulsive. This extension is also nontrivial since repulsive terms lead to complex static fields within the SPA and a full CSPA treatment in all variables cannot be straightforwardly applied. In this work we shall show that the repulsive static fields can be accurately treated in the stationary-phase approximation, for *arbitrary* values of the attractive static fields, except for very low temperatures in special situations. This allows us to develop a partial CSPA treatment where large-amplitude fluctuations are restricted to the variables associated with attractive terms, but where the RPA corrections contain the effects of the repulsive forces. This provides in fact a justification of more phenomenological treatments of the dipole Hamiltonian, where statistical fluctuations are restricted to the pairing and quadrupole shape deformations. The present work extends considerably Ref. [23], where just a pure repulsive interaction without attractive terms was studied. We also examine the case, not previously considered, where the repulsive terms modify the mean field, which requires a special adjustment of the integration path within the SPA.

In Sec. II we discuss in detail the formal treatment of repulsive forces within the SPA and CSPA. The RPA correction to the SPA is evaluated exactly. We then examine in Sec. III models containing both attractive and repulsive terms, where the accuracy of the present methods and the effects of repulsive terms on the generalized thermal RPA frequencies and thermodynamic distributions are analyzed. An important outcome is that repulsive terms may enhance tunneling effects between mean-field minima, and this can be correctly described by the CSPA within its range of applicability. We also examine repulsive terms that modify the mean field, including a particular case where the SPA is exact, to set limits to the validity of the stationary-phase approximation for the static repulsive variables. Finally, conclusions are drawn in Sec. IV.

II. FORMALISM

A. SPA in the presence of repulsive forces

We consider a general fermionic Hamiltonian containing just one- and two-body terms. Within a finite configuration space, it can be always written in the separable form [3]

$$H = H_0 - \frac{1}{2}\sum_\nu v_\nu Q_\nu^2, \tag{1}$$

where H_0 and Q_ν are Hermitian one-body (one particle or one quasiparticle) operators. Using the HS transformation [2] and separating explicitly the attractive ($v_\nu > 0$) and repulsive

($v_\nu<0$) terms in Eq. (1), the grand canonical (GC) partition function can be cast as the path integral

$$Z=\mathrm{Tr}\,\exp[-\beta H']=\int D[x]D[y]\mathrm{Tr}\,\hat{T}\,\exp\left\{-\int_0^\beta dt\,H'[x(t),y(t)]\right\},\tag{2}$$

where $H'=H-\mu N$, $\hat{T}$ denotes time ordering, and

$$H'(x,y)=H_0-\mu N+\sum_{\nu,v_\nu>0}\left(\frac{x_\nu^2}{2v_\nu}-x_\nu Q_\nu\right)-\sum_{\nu,v_\nu<0}\left(\frac{y_\nu^2}{2|v_\nu|}+y_\nu Q_\nu\right)\tag{3}$$

is a one-body operator. The integral over the variables y associated with the repulsive terms is to be taken along the *imaginary* axis (we assume $\beta>0$).

In the SPA, just the time independent paths in Eq. (2) are considered. This leads to

$$Z_{\rm SPA}=\int_{-\infty}^{\infty}d(x)\int_{-\infty}^{\infty}d(y')Z(x,y_0+iy'),\tag{4}$$

$$Z(x,y)=\mathrm{Tr}\,\exp[-\beta H'(x,y)]=\exp[-\beta\mathcal{F}(x,y)],\tag{5}$$

$$d\begin{pmatrix}x\\ y'\end{pmatrix}=\prod_{\nu,v_\nu\gtrless 0}\left(\frac{\beta}{2\pi|v_\nu|}\right)^{1/2}\begin{pmatrix}dx_\nu\\ dy'_\nu\end{pmatrix},$$

where y_0 is a set of real constants, arbitrary in principle, which determine the integration path. If the operators Q_ν commute with each other and with $H_0-\mu N$, Eq. (4) is *exact and independent of* y_0 for all β. In the general case, it becomes exact and independent of y_0 for $\beta\to 0$ (i.e., at high temperatures $T=1/k\beta$) up to order β, and the shift y_0 can be employed to optimize the SPA at low temperatures and to evaluate the integral over y' in the stationary-phase approximation, as discussed below.

The stationary points of the potential $\mathcal{F}(x,y)$ are determined by the self-consistent Hartree equations

$$x_\nu=v_\nu\langle Q_\nu\rangle_{x,y}\equiv v_\nu\mathrm{Tr}\{\exp[-\beta H'(x,y)]Q_\nu\}/Z(x,y),\tag{6}$$

$$y_\nu=-|v_\nu|\langle Q_\nu\rangle_{x,y}\,.\tag{7}$$

At a real solution of Eqs. (6) and (7), $\mathcal{F}(x,y)$ becomes the Hartree grand potential $\mathcal{F}_H$, which, in the pure attractive case where all $v_\nu>0$, is an *upper* bound to the exact grand potential $\mathcal{F}$, implying $Z_H\equiv e^{-\beta\mathcal{F}_H}\leqslant Z=e^{-\beta\mathcal{F}}$, while in the repulsive case where all $v_\nu<0$, it is a *lower* bound, implying $Z_H\geqslant Z$ (see Appendix A). For $x\to\pm\infty$, $\mathcal{F}(x,y)\to\infty$ and along the real x_ν axis $\mathcal{F}(x,y)$ will possess one or several minima (degenerate when symmetries of H are broken) determined by Eq. (6). In small finite systems, these minima will be normally flat, particularly in transitional regions, and the SPA integral over x will take into account the large-amplitude thermal fluctuations around these solutions.

On the other hand, along the real y_ν axis $\mathcal{F}(x,y)\to-\infty$ for $y_\nu\to\pm\infty$ and the real solution of Eq. (7) corresponds to a *maximum*, i.e., a minimum of $Z(x,y)$. For fixed x, this real solution is *unique*, as $\partial^2\mathcal{F}(x,y)/\partial y_\nu^2<0$ for real x,y [see Eq. (9) below]. However, along the imaginary axis, $\mathrm{Re}[Z(x,y_0+iy')]$ has a maximum at $y'=0$ for *any* real y_0, although it may exhibit oscillatory behavior and sign changes. The integral over y' represents rather a type of projection that will decrease the partition function. For a given x, the oscillations disappear or become attenuated if y_0 is chosen as the real solution of Eq. (7), in which case $\mathrm{Im}[Z(x,y_0+iy')]$ is also stationary at $y'=0$ and the inner integral in Eq. (4) can be evaluated in the saddle-point approximation. This leads to

$$Z_{\rm SPA}\approx\int_{-\infty}^{\infty}d(x)Z(x,y_0(x))C_0(x),\tag{8}$$

where $y_0(x)$ is the real solution of Eq. (7) for fixed x and

$$C_0(x)=\mathrm{Det}\left[-|v_\nu|\frac{\partial^2\mathcal{F}(x,y)}{\partial y_\nu\partial y_{\nu'}}\bigg|_{y=y_0(x)}\right]^{-1/2}=\mathrm{Det}\left[\delta_{\nu\nu'}+|v_\nu|\sum_{k,k'}\langle k|Q_\nu|k'\rangle\times\langle k'|Q_{\nu'}|k\rangle F_{kk'}\right]^{-1/2},\tag{9}$$

$$F_{kk'}=\frac{f_k-f_{k'}}{\lambda_{k'}-\lambda_k}(k\neq k'),\quad F_{kk}=\beta f_k(1-f_k),$$

with $|k\rangle,\lambda_k$ the single-particle eigenstates and eigenvalues of $H'(x,y_0(x))$ and f_k the Fermi occupation probabilities (assuming a GC ensemble). The labels ν,ν' in Eq. (9) are restricted to the repulsive terms. Note that $F_{kk'}>0$ for $\beta>0$ (with $F_{kk'}\to F_{kk}$ if $\lambda_k\to\lambda_{k'}$) so that $C_0(x)<1$. If $[H'(x,y),N]\neq 0$, $\Sigma_{k\neq k'}\to\frac{1}{2}\Sigma'_{k\neq k}$, where the prime indicates the sum over the extended quasiparticle space of doubled dimension [9].

Equation (8) will practically coincide with the full integral (4), except for very low temperatures [where, excluding the commuting case, Eq. (4) is not accurate either] and will therefore be exact for $T\to\infty$. The factor $C_0(x)$ *decreases* the partition function, improving the Hartree result $Z(x,y_0(x))$, although its effect on the normalized distribution over x [the integrand in Eq. (8) is now positive definite and can be interpreted as a thermodynamic probability] will be normally quite small. If, for $v_\nu<0$, $\langle Q_\nu\rangle_{x,0}=0\ \forall x$, the repulsive terms do not modify the Hartree mean field and $y_0(x)=0$, in which case their only effect at the SPA level is the factor $C_0(x)$.

B. RPA correlations

Further effects of the repulsive terms will appear only at low temperatures, where quantum fluctuations become important. The energy $-\partial\ln Z/\partial\beta$ obtained from Eq. (8) will approach just the Hartree energy for low T, omitting further correlations that will be sensitive to the presence of repulsive forces. The time-dependent variables in Eq. (2) can be expanded as

$$x_\nu(t)=\sum_{m=-\infty}^{\infty} x_\nu^m e^{i\omega_m t}, \quad \omega_m=2\pi m/\beta \tag{10}$$

[similarly for $y_\nu(t)$] and Eq. (2) can be written as an integral over the coefficients x_ν^m, y_ν^m. In the CSPA [16,17] the integrals over the *static* components x_ν^0 are fully retained, while those over $x_\nu^{m\neq 0}$, representing the time-dependent or quantum fluctuations, are evaluated in the saddle-point approximation. The small amplitude quantum fluctuations are thus incorporated. In the present situation, we integrate in addition over $y_\nu^{m\neq 0}$ *and* y_ν^0 in the saddle-point approximation. The result, obtained after an expansion of the logarithm of the propagator in Eq. (2) up to second order in $x_\nu^{m\neq 0}, y_\nu^m$, is

$$Z_{\rm CSPA}=\int_{-\infty}^{\infty} d(x) Z(x,y_0(x)) C_0(x) C_{\rm RPA}(x), \tag{11}$$

$$C_{\rm RPA}(x)=\prod_{m=1}^{\infty} {\rm Det}\left[\delta_{\nu\nu'}-v_\nu \times\sum_{k\neq k'}\frac{\langle k|Q_\nu|k'\rangle\langle k'|Q_{\nu'}|k\rangle(f_k-f_{k'})}{i\omega_m+\lambda_{k'}-\lambda_k}\right]^{-1}, \tag{12}$$

where ν,ν' run over the full set of operators. Equation (12) can be evaluated exactly in terms of the generalized RPA frequencies $\omega_\alpha(x)$, defined as the roots [16]

$${\rm Det}\left[\delta_{\nu\nu'}-v_\nu\sum_{k\neq k'}\frac{\langle k|Q_\nu|k'\rangle\langle k'|Q_{\nu'}|k\rangle(f_k-f_{k'})}{-\omega_\alpha+\lambda_{k'}-\lambda_k}\right]=0,$$

which become the conventional thermal Hartree RPA frequencies if x is a solution of Eq. (6). Their total number with a definite sign is equal to the total number of pairs $k<k'$. Defining in addition $\lambda_\alpha(x)\equiv\lambda_{k'}-\lambda_k$ $(k<k')$, Eq. (12) becomes

$$C_{\rm RPA}(x)=\prod_{m=1}^{\infty}\prod_\alpha \frac{\omega_m^2+\lambda_\alpha^2(x)}{\omega_m^2+\omega_\alpha^2(x)} \tag{13}$$

$$=\prod_\alpha \frac{\sinh[\frac{1}{2}\beta\lambda_\alpha(x)]/\lambda_\alpha(x)}{\sinh[\frac{1}{2}\beta\omega_\alpha(x)]/\omega_\alpha(x)}, \tag{14}$$

where Euler's formula has been applied for evaluating the product over m [20]. As $\frac{1}{2}\sinh^{-1}(\frac{1}{2}\beta\omega)=e^{-\beta\omega/2}/(1-e^{-\beta\omega})$ is the oscillator partition function, $C_{\rm RPA}(x)$ is proportional to the quotient between the partition function of independent RPA bosons with energies $\omega_\alpha(x)$ to that of uncorrelated pairs with energies $\lambda_\alpha(x)$, considered as bosons. The additional factors $\lambda_\alpha^{-1}(x),\omega_\alpha^{-1}$ arise due to the exclusion of the $m=0$ term in Eq. (13) and make Eq. (14) positive definite even if, for some α,x, $\omega_\alpha(x)=0$ (as, for instance, in Goldstone modes) or if $\omega_\alpha(x)$ becomes *imaginary*, provided in this case $|\beta\omega_\alpha(x)|<2\pi$.

For high T, $C_{\rm RPA}(x)\to 1$ in a finite space. The RPA corrections become important for low T (i.e., below the relevant mean-field critical temperature T_c) and will contain the most significant effects of the repulsive terms on the normalized distribution over x. Some of the lowest frequencies $\omega_\alpha(x)$ will normally become imaginary (or complex) for $T<T_c$ for x away from a stable Hartree solution, in which case Eq. (11) will not be applicable in the regions where $\beta^2\omega^2(x)\leqslant -4\pi^2$, which will arise below a certain temperature $T_c'<T_c$. For $T<T_c'$, $C_{\rm RPA}(x)$ is no longer positive definite and exhibits poles. This indicates the failure of the saddle-point approximation for $x_\nu^{m\neq 0}$ in these regions due to the onset of large-amplitude quantum fluctuations [16]. Note also that the CSPA is not directly applicable to the full SPA treatment (4), as the ensuing energies λ_k will normally become complex for sufficiently large y' and $C_{\rm RPA}(x,y_0+iy')$ is not necessarily positive definite (at any temperature).

III. APPLICATION

We consider a model space of 2Ω single-particle states $|p\nu\rangle$, $p=1,\ldots,\Omega$, $\nu=\pm 1$, and define the fermionic quasispin operators [24]

$$J_z=\frac{1}{2}\sum_{p,\nu}\nu c^\dagger_{p\nu}c_{p\nu}, \quad J_\nu=J_x+i\nu J_y=\sum_p c^\dagger_{p\nu}c_{p-\nu}, \tag{15}$$

which satisfy the standard SU(2) commutation relations. Any two-body quasispin Hamiltonian can be written, after a suitable rotation, as

$$H=\sum_{i=x,y,z}\varepsilon_i J_i - v_i J_i^2/\Omega. \tag{16}$$

The linearized SPA Hamiltonian and the partition function (5) become $[\boldsymbol{r}\equiv(x,y,z)]$

$$H(\boldsymbol{r})=\sum_i \Omega r_i^2/4v_i+\lambda_i J_i, \quad \lambda_i=\varepsilon_i-r_i, \tag{17}$$

$$Z(\boldsymbol{r})={\rm Tr}\exp[-\beta H(\boldsymbol{r})] =\exp\left[-\beta\Omega\sum_i\frac{r_i^2}{4v_i}\right]\{2\cosh[\beta\gamma\lambda]\}^{\Omega/2\gamma}, \tag{18}$$

where $\lambda=(\lambda_x^2+\lambda_y^2+\lambda_z^2)^{1/2}$ and $\gamma=1/4$ in the GC ensemble and $\gamma=1/2$ in the restricted SU(2) canonical ensemble (see Appendix B). Equation (18) holds also for complex λ_i. The Hartree equations become

$$r_i=2v_i\langle J_i\rangle_{\boldsymbol{r}}/\Omega=-v_i\tanh[\beta\gamma\lambda]\frac{\lambda_i}{\lambda}, \tag{19}$$

which are independent of Ω, and the ensuing Hartree partition function $Z(\boldsymbol{r_0})$ yields the leading order of the exact partition function (B3) for $\Omega\to\infty$ and fixed v_i.

A. Lipkin model

We consider first the Hamiltonian

$$H=\varepsilon J_z - vJ_x^2/\Omega+v'J_y^2/\Omega. \tag{20}$$

For $v=v'=\Omega V$, H becomes the well-known Lipkin Hamiltonian [24]

$$H=\varepsilon J_z-V(J_x^2-J_y^2)=\varepsilon J_z-\tfrac{1}{2}V(J_+^2+J_-^2), \qquad (21)$$

which contains an attractive plus a repulsive term. We set in what follows $v>0$, $v'>0$. The SPA partition function is

$$Z_{\rm SPA}=\frac{\beta\Omega}{4\pi(vv')^{1/2}}\int_{-\infty}^{\infty}dx\int_{-\infty}^{\infty}dy'Z(x,iy') \qquad (22)$$

$$\approx\left(\frac{\beta\Omega}{4\pi v}\right)^{1/2}\int_{-\infty}^{\infty}dx\ Z(x,0)C_0(x), \qquad (23)$$

$$C_0(x)=\{1+v'\tanh[\beta\gamma\lambda(x)]/\lambda(x)\}^{-1/2},$$

$$\lambda(x)=(\varepsilon^2+x^2)^{1/2}, \qquad (24)$$

where $Z(x,y)$ denotes Eq. (18) for $\boldsymbol{r}=(x,y,0)$. The present repulsive term does not affect the mean field ($\langle J_y\rangle_{x,0}=0$), so that $y_0(x)=0\ \forall\ x$.

The difference between Eqs. (22) and (23) is negligible for all T, *including* the $T\to 0$ limit, and also for all $v'>0$, *including* $v'\gg v$ (it is less than 2% in all cases for $\Omega=10$). For $v=v'$, we can recast Eq. (22) explicitly as a one-dimensional integral writing $x=s\cosh\phi$, $y'=s\sinh\phi$, for $|x|>|y'|$, and conversely for $|x|<|y'|$, such that $s^2=|x^2-y'^2|$, obtaining

$$Z_{\rm SPA}=\frac{\beta\Omega}{2\pi v}\int_0^{\infty}s\ ds\ K_0\left(\frac{\beta\Omega s^2}{4v}\right)e^{\beta\Omega s^2/4v}[Z(s,0)+Z(0,is)],$$

where $K_0(u)=2\int_0^{\infty}e^{-u\cosh 2\phi}d\phi$ is the modified Bessel function of the second kind. Although for $s>\varepsilon$, $Z(0,is)$ (the contribution from the region $|y'|>|x|$) can be negative, its magnitude is negligible in comparison with $Z(s,0)$ and no cancellation effects arise. The difference with Eq. (23) is less than 0.06% for all $T>0$ in the case of Fig. 1.

The Hartree mean field is the same as for $v'=0$. Equation (19) becomes

$$x=vx\ \tanh[\beta\gamma\lambda(x)]/\lambda(x) \qquad (25)$$

and possesses, in addition to the normal solution $x=0$, a ‘‘deformed’’ solution $x=\pm x_0$ for $v>\varepsilon$ and $T<T_c$, which breaks the parity symmetry (i.e., $\langle J_x\rangle_{x_0}\neq 0$; in the exact case, $[H,e^{i\pi J_z}]=0$ and $\langle J_x\rangle=0$) and leads to the absolute maxima of $Z(x,0)$ for $T<T_c$. The second-order deformed to normal Hartree transition at

$$T_c=2\gamma\varepsilon/\ln\left(\frac{v+\varepsilon}{v-\varepsilon}\right) \qquad (26)$$

becomes, however, considerably smooth for small Ω in the exact partition function, and this smoothing is accurately described by the SPA. In the thermal Hartree-Fock (HF) approximation, Eqs. (B10) and (B11), the final effect of exchange terms is the renormalization $v\to v(1-1/\Omega)$ in the Hartree expressions. The repulsive term leads in the HF approximation to an essentially constant shift in the energy

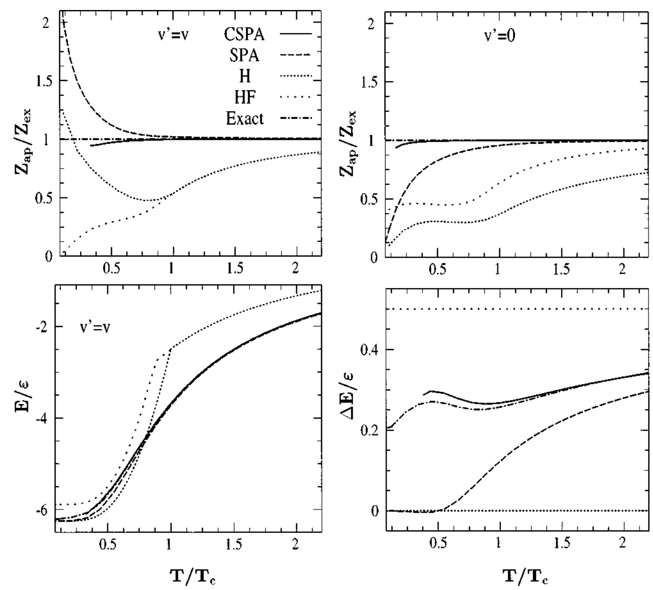

FIG. 1. Top: quotient between approximate and exact partition functions for the Hamiltonian (20), for $v/\varepsilon=2$, $\Omega=10$, and $v'=v$ (left) and $v'=0$ (right). Bottom: average energy for $v'=v$ (left) and the difference $\Delta E=E(v'=v)-E(v'=0)$ (right) as a function of temperature. In all panels, SPA denotes Eq. (23), which is undistinguishable from Eq. (22), CSPA denotes Eq. (11), and H and HF denotes the thermal Hartree and Hartree-Fock results. The Hartree critical temperature is $T_c/\varepsilon=0.91$.

[strictly constant for $\gamma=1/2$; see Eq. (B13)], which does not alter the mean field picture and equations.

We examine now the RPA correlations. There is a single collective RPA frequency $\omega(x)$ and Eq. (11) becomes [see Eq. (B7)]

$$C_{\rm RPA}(x)=\frac{\sinh[\frac{1}{2}\beta\lambda(x)]\omega(x)}{\sinh[\frac{1}{2}\beta\omega(x)]\lambda(x)}, \qquad (27)$$

$$\omega^2(x)=\lambda^2(x)\{1-v\varepsilon^2\tanh[\beta\gamma\lambda(x)]\lambda^3(x)\}$$
$$\times\{1+v'\tanh[\beta\gamma\lambda(x)]/\lambda(x)\} \qquad (28)$$

$$\approx 4vv'\lambda^2(x){\rm Det}\left[\frac{\partial^2\mathcal{F}(x,iy')}{\partial\eta_i\partial\eta_j}\right]_{y'=0}, \qquad \eta=(x,y'), \qquad (29)$$

where $\mathcal{F}=-T\ln Z(x,iy')/\Omega$ [equality in Eq. (29) would strictly hold if the last term in Eq. (B9), arising from the diagonal term $\nu=\nu'$ in Eq. (B8), were omitted in the second derivative; this term vanishes for $T\to 0$]. In particular,

$$\omega^2(0)=[\varepsilon-v\ \tanh(\beta\gamma\varepsilon)][\varepsilon+v'\tanh(\beta\gamma\varepsilon)], \qquad (30)$$

$$\omega^2(x_0)=x_0^2(1+v'/v) \quad (T<T_c), \qquad (31)$$

where x_0 is the symmetry-breaking solution of Eq. (25), are the conventional thermal Hartree RPA frequencies (squared). Note that $\omega^2(0)<0$ for $T<T_c$ (and $v>\varepsilon$), indicating the instability of the normal Hartree solution. For arbitrary x, we have $\omega^2(x)>0\ \forall x$ for $T>T_c$ or $v<\varepsilon$, whereas for $v>\varepsilon$ and $T<T_c$, $\omega^2(x)<0$ in the vicinity of $x=0$, corresponding ap-

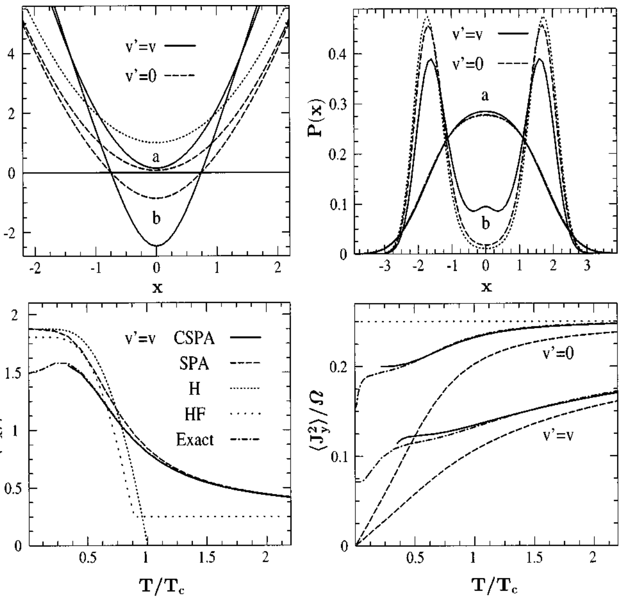

FIG. 2. Top left: the squared RPA frequency, Eq. (28), as a function of x (in units of ε) for the cases of Fig. 1 and (a) $T=1.1T_c$ and (b) $T=0.3T_c$. The dotted line depicts the squared uncorrelated pair energy $\lambda^2(x)$. Top right: corresponding normalized distribution $P(x)\propto Z(x)C_0(x)C_{\rm RPA}(x)$ at the same temperatures. The dotted line depicts the main SPA contribution $P(x)\propto Z(x)$ (independent of v'). Bottom: averages of J_x^2 and J_y^2.

proximately to the region where $\mathcal{F}(x,0)$ has a negative curvature. The breakdown of the CSPA occurs at the temperature $T_c'<T_c$ determined by

$$\beta^2\omega^2(0)=-4\pi^2 \tag{32}$$

and indicates the onset for $T<T_c'$ of large-amplitude tunneling across the barrier between the two degenerate deformed mean-field minima. The equation $\beta^2\omega^2(0)=-4\pi^2m^2$ determines the temperature for the breakdown of the Gaussian approximation for x^m in Eq. (10), reflected in the appearance of the mth pole in $C_{\rm RPA}(x)$ (note that for $m=0$, this equation determines the critical temperature T_c).

The repulsive term increases $|\omega(x)|$ and hence $|\omega(0)|$, increasing thus the breakdown temperature T_c' [for $v'\to\infty$, $T_c'\to T_c$, with $T_c-T_c'=O(v'^{-1})$]. This reflects the enhancement of tunneling effects by the repulsive term (see below). Note also that the CSPA is not applicable to the full SPA treatment (4), as $\lambda(x,iy')=(\varepsilon^2+x^2-y'^2)^{1/2}$ acquires arbitrary large imaginary values for large y', and $C_{\rm RPA}(x,iy')$ will exhibit poles at any temperature.

Numerical results shown in Figs. 1 and 2 correspond to the ensemble with $\gamma=1/2$. The CSPA partition function (11) is almost exact for $T>T_c'$. The accuracy for $v'=v$ is similar to that for the pure attractive case $v'=0$, but T_c' is higher (for $v=2\varepsilon$, $T_c'/\varepsilon=0.26$ for $v'=v$ and $T_c'/\varepsilon=0.16$ for $v'=0$). The SPA is also quite accurate for $T>T_c$, where the factor $C_0(x)$ accounts for the most important effects of the repulsive term, although for low T the SPA approaches just the Hartree results, which are independent of v'. In the case depicted, the $T=0$ Hartree energy lies slightly below the exact ground-state energy for $v'=v$, which implies $Z_{\rm SPA}>Z_{\rm ex}$ and $E_{\rm SPA}<E_{\rm ex}$ for low T. In contrast, all approximations are lower bounds to $Z_{\rm ex}$ for $v'=0$. Nevertheless, the detailed increase in the average energy due to the repulsive term is accurately described only by the CSPA (for $T>T_c'$). Note that the HF approximation predicts just a constant increase (it is zero at the Hartree level), which is too large. This shift makes the $T=0$ HF energy an upper bound, but the Hartree energy lies in this case closer to the exact energy. We also mention that CSPA results for the level density (evaluated in the saddle-point approximation) are undistinguishable from the exact ones.

The RPA frequency and the final CSPA distribution are depicted in Fig. 2. For $T>T_c'$, $C_{\rm RPA}(x)>1$ when $\omega^2(x)<\lambda^2(x)$ (and vice versa), so that, in particular, $C_{\rm RPA}(x)>1$ when $\omega(x)$ is imaginary. The RPA correction will then increase the normalized distribution $[\int_{-\infty}^{\infty}P(x)dx=1]$ near the origin for $T<T_c$, particularly near the breakdown temperature. This effect is strongly enhanced by the repulsive term, due to the increase in $|\omega(0)|$ and the fact that for $v'>0$, $\omega^2(x)>\lambda^2(x)$ and $C_{\rm RPA}(x)<1$ for large x [in the case depicted, $C_{\rm RPA}(x)<1$ already at the mean-field solution for $T<T_c$]. Thus, at the RPA level the repulsive term lowers the potential barrier between the mean-field wells, favoring tunneling. The factor $C_0(x)$ decreases the partition function, but its effect on the normalized distribution is very small. In the pure attractive case $v'=0$, $\omega^2(x)<\lambda^2(x)$, and $C_{\rm RPA}(x)>1$ $\forall x$. The variation of $C_{\rm RPA}(x)$ is here smaller and its main effect is to decrease the partition function, without altering significantly the distribution shape. Note that the RPA energy correction for fixed x is essentially $E_b[\omega(x)]-E_b[\lambda(x)]$, where $E_b(\omega)=\frac{1}{2}\omega\coth(\beta\omega/2)$ is the average bosonic energy, and it is positive when $C_{\rm RPA}(x)<1$ (and vice versa). For $v'=0$ it is negative for all x, while for $v'=v$, it is negative near $x=0$ and positive otherwise.

The RPA corrections will have a visible effect on the averages (Fig. 2, bottom)

$$\langle J_i^2\rangle=\Omega\beta^{-1}\partial\,\ln Z/\partial v_i,\quad i=x,y, \tag{33}$$

which represent the total strength of the operators J_x,J_y. The CSPA results are again almost exact above the breakdown, while the SPA is quite reliable for $T>T_c$. The repulsive term decreases $\langle J_x^2\rangle$ for low T and this is correctly described only by the CSPA (the exact result for $v'=0$ is close to the SPA). It also decreases $\langle J_y^2\rangle$ [note that in the HF approximation, $\langle J_y^2\rangle=\Omega/4$ for all T and $v'\geqslant 0$, while $\langle J_x^2\rangle=\Omega/4$ for $T>T_c$ (B13)]. At the CSPA breakdown, the exact values of $\langle J_x^2\rangle$ and $\langle J_y^2\rangle$ exhibit a rather sharp decrease as T decreases. In this region the ground-state contribution becomes dominant in the expectation value and the tunneling between the two mean-field wells becomes important. The higher breakdown temperature for $v'=v$ reflects the larger splitting between the exact ground and first excited states of H (it is 0.27ε for $v'=v=2\varepsilon$ and 0.037ε for $v'=0$). This is in agreement with the decrease in the potential barrier between the mean-field wells given by the CSPA.

B. Repulsive term modifying the mean field

We consider now

$$H=\varepsilon J_z - v J_x^2/\Omega + v' J_z^2/\Omega, \tag{34}$$

where we set $v \geqslant 0$, $v' \geqslant 0$. The repulsive term will in this case modify the mean field, leading to a renormalization of the unperturbed single-particle energy ε. This effect will depend nevertheless on temperature and, within the SPA, also on the deformation x.

It is instructive to consider first the case $v=0$, where the SPA is *exact*, in order to test Eq. (8). The exact energies are obviously $\varepsilon M + v' M^2/\Omega$ and the ground state corresponds to $M=-\frac{1}{2}\Omega$ for $v' < v'_c = \varepsilon\Omega/(\Omega-1)$ and to $M=-[\frac{1}{2}(\Omega\varepsilon/v'+1)]$ for $v'>v'_c$, with $M=0$ for $v'>\Omega\varepsilon$ (we assume Ω even). It undergoes $\Omega/2$ transitions $M\rightarrow M+1$ as v' increases from 0 to $\Omega\varepsilon$, becoming degenerate for $v'>v'_c$. The SPA partition function is

$$Z_{\rm SPA}=\left(\frac{\beta\Omega}{4\pi v'}\right)^{1/2}\int_{-\infty}^{\infty} dz'\, Z(z_0+iz'), \tag{35}$$

where $Z(z)$ denotes Eq. (18) for $\boldsymbol{r}=(0,0,z)$ and is exact and *independent* of z_0. The RPA corrections vanish ($C_{\rm RPA}=1$). The saddle-point approximation to Eq. (35) reads

$$Z_{\rm SPA}\approx Z(z_0)[1+v'\beta\gamma(1-z_0^2/v'^2)]^{-1/2}, \tag{36}$$

with z_0 determined from the Hartree equation

$$z_0 = v' \tanh[\beta\gamma(\varepsilon - z_0)]. \tag{37}$$

For $v'>0$, $0<z_0<\varepsilon$, so that the repulsive term decreases the final single-particle energy $\lambda_z=\varepsilon-z_0$ [cf. Eq. (17)]. For $T\rightarrow 0$, $z_0\rightarrow \min(v',\varepsilon)$. The transition at $v'=\varepsilon$ reflects the onset of ground states with $|M|<\frac{1}{2}\Omega$, but no further transition occurs in the Hartree approach as v' or T increases (z_0 vanishes as $v'\beta\gamma\varepsilon$ for $T\rightarrow\infty$). Instead, for $v'>\varepsilon$ and $T\rightarrow 0$, $\langle J_z\rangle_{z_0}\rightarrow -\Omega\varepsilon/2v'$, which represents the classical limit of *continuous* M of the exact ground state. The ensuing Hartree energy $\langle H\rangle_{z_0}$ is exact in this limit only for integer $\Omega\varepsilon/2v$, lying otherwise *below* the exact energy. As seen in Fig. 3, the Hartree partition function $Z(z_0)$ provides a rather poor estimate. This is also the case in the HF approximation [where the final effect is again the replacement $v'\rightarrow v'(1-1/\Omega)$ plus a constant shift in the energy].

The approximation (36) is nevertheless practically exact for all T, *except* for $T\rightarrow 0$ when $v'>\varepsilon$. This is apparent as the energy obtained from Eq. (36) approaches the Hartree result in this limit. For $T\rightarrow 0$ and $v'>\varepsilon$ ($T<0.1\varepsilon$ in the case of Fig. 4) the exact SPA integral (35) *projects* from the trace the matrix element with the correct integer value of M and the energy obtained from Eq. (35) does not approach the Hartree energy. In this limit cancellations between positive and negative values of the integrand along the integration path take place and the saddle-point approximation for the static repulsive variables fails. Note that $\mathrm{Re}[Z(z_0+iz')]$ has a maximum at $z'=0$ for *any* real choice of z_0 (Fig. 3), but becomes highly oscillating at low T if z_0 is different from the Hartree solution. Only for $T\rightarrow 0$ and $v'>\varepsilon$ do the oscillations, though attenuated, subsist even for this point.

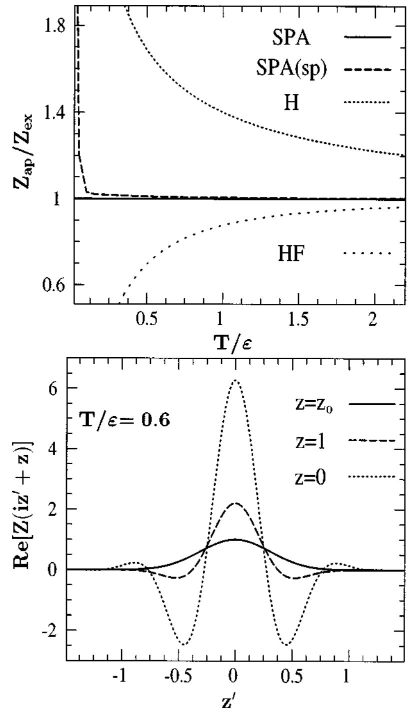

FIG. 3. Top: quotient between approximate and exact partition functions for the Hamiltonian (34), for $v=0$, $v'/\varepsilon=2$, and $\Omega=10$. SPA denotes the full integral (35), exact in the present case, SPA(sp) the saddle-point approximation (36), and H and HF the thermal Hartree and Hartree-Fock results. Bottom: real part of the integrand in Eq. (35) [scaled to $Z(z_0)$] for different values of the shift z (in units of ε). $z_0=0.62$ denotes the Hartree solution.

In the full case $v>0$, $v'>0$, the SPA becomes

$$Z_{\rm SPA}=\frac{\beta\Omega}{4\pi(vv')^{1/2}}\int_{-\infty}^{\infty}dx\int_{-\infty}^{\infty}dz'\,Z(x,z_0+iz') \tag{38}$$

$$\approx\left(\frac{\beta\Omega}{4\pi v}\right)^{1/2}\int_{-\infty}^{\infty}dx\; Z(x,z_0(x))C_0(x), \tag{39}$$

where $Z(x,z)$ corresponds to $\boldsymbol{r}=(x,0,z)$ in Eq. (18). The Hartree equations are

$$x = vx\,\tanh[\beta\gamma\lambda(x,z)]/\lambda(x,z), \tag{40}$$

$$z = v'(\varepsilon - z)\tanh[\beta\gamma\lambda(x,z)]/\lambda(x,z), \tag{41}$$

with $\lambda(x,z)=[(\varepsilon-z)^2+x^2]^{1/2}$, and $z_0(x)$ in Eq. (39) is the real solution of Eq. (41) for fixed x. This implies an x-dependent "unperturbed" single-particle energy $\lambda_z(x)=\varepsilon-z_0(x)$.

Let us examine first the solutions of the combined system (40) and (41). If a symmetry-breaking solution $x=\pm x_0\neq 0$ exists, Eq. (41) yields $z=(\varepsilon-z)v'/v$, i.e., $z=v'\varepsilon/(v+v')$, *independent* of temperature. This implies $\lambda_z\equiv\varepsilon-z=\varepsilon v/(v+v')$. The symmetry-breaking solution will then exist for $v>\lambda_z$, i.e., $v+v'>\varepsilon$, and will be similar to that of the Lipkin model for $\varepsilon=\lambda_z$, with a transition to the normal

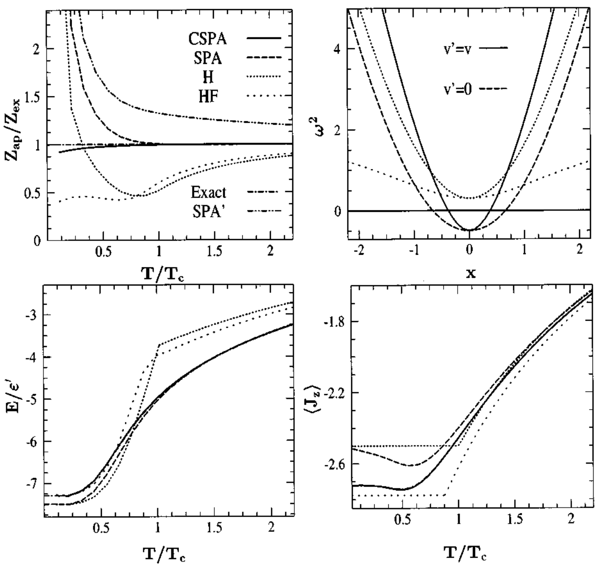

FIG. 4. Top left: quotient between approximate and exact partition functions for $v'=v=\varepsilon$ in Eq. (34) and $\Omega=10$. SPA denotes Eq. (39), which is undistinguishable from Eq. (38), while SPA′ denotes the result neglecting $C_0(x)$ in Eq. (39). Top right: squared RPA frequency (42), for $T=0.3T_c$. The result for $v'=0$ in Eq. (42) is also shown. The thick dotted line depicts the uncorrelated pair energy $\lambda^2(x,z_0(x))$, the light dotted line $\lambda_z^2=[\varepsilon-z_0(x)]^2$. Bottom: average energy and J_z (ω, x, and E are in units of $\varepsilon'=\varepsilon/2$). The CSPA results overlap with the exact ones (same line conventions as top left panel).

phase at $T=T_c$ [given by Eq. (26) for $\varepsilon=\lambda_z$]. For $T>T_c$ or $v+v'<\varepsilon$, x vanishes and z becomes again temperature dependent, being identical to the case $v=0$, previously discussed. If $v'>\varepsilon$, the symmetry-breaking solution exists for *any* $v>0$ (for $T<T_c$). The present repulsive term favors thus the onset of the symmetry-breaking phase through the decrease in λ_z. For $v=v'$, $\lambda_z=\varepsilon/2$.

In Eq. (39), x is not restricted to the self-consistent solution and $z_0(x)$ will depend on both x and T. The effect is again to decrease $\lambda_z(x)$ for small x and low T [for $T\to 0$, $\lambda_z(0)\to 0$ for $v'>\varepsilon$] while for $|x|\to\infty$, $z_0(x)$ vanishes. The difference between Eqs. (38) and (39) is again negligible, even for $T\to 0$ if $v+v'>\varepsilon$ [and if z_0 in Eq. (38) is close to the saddle point $z_0(x)$] since the residual effects of the repulsive term on the deformed ground state are small [for fixed x, the difference between the integrand in Eq. (39) and the inner integral in Eq. (38) decreases as $|x|$ increases]. In any case, Eq. (38) is no longer exact for $T\to 0$.

The factor $C_{\rm RPA}(x)$ has the same form (27), with

$$\omega^2(x)=\lambda^2(x)+\frac{v'x^2-v[\varepsilon-z_0(x)]^2}{\lambda(x)}\tanh[\beta\gamma\lambda(x)], \qquad (42)$$

where $\lambda(x)\equiv\lambda(x,z_0(x))$ [$\omega^2(x)$ is approximately given again by Eq. (29) with $y'\to z'$]. At the symmetry-breaking solution $x=\pm x_0$, $\omega^2(x_0)=x_0^2(1+v'/v)$, which is identical to Eq. (31), but the behavior differs for other x. Again, for $T>T_c$, $\omega^2(x)>0$ $\forall x$, whereas for $T<T_c$, $\omega^2(0)<0$ and $\omega(x)$ becomes imaginary in the vicinity of the origin, as depicted in Fig. 4. However, the effect of v' in Eq. (42) is to increase $\omega^2(x)$ for $x\neq 0$, without altering $\omega(0)$, so that it will not increase the breakdown temperature T'_c, determined from Eq. (32) (in the case depicted, $T'_c/\varepsilon'=0.1$). Moreover, T'_c will in this case *decrease* with increasing v' since $\varepsilon-z_0(0)$ and hence $\omega(0)$ will decrease, *vanishing* for $v'\to\infty$ [in this limit $T'_c=O(v'^{-2})$]. Accordingly, the increase in the normalized distribution near the origin due to $C_{\rm RPA}(x)$ will be small (similar in the case depicted to that for $v'=0$ in Fig. 2). Tunneling effects become suppressed by the present repulsive term, as confirmed by the tiny splitting between the exact ground and first excited states (just $0.001\varepsilon'$ in the case depicted).

The CSPA equation (11) is again practically exact for thermodynamic quantities above the breakdown temperature, as seen in Fig. 4, whereas the SPA in the form (39) remains quite accurate for $T>T_c$. In this case we have depicted the average of J_z, which remains constant in the symmetry-breaking phase in the Hartree and HF approaches. The CSPA reproduces with extreme accuracy the detailed low-temperature behavior. The $T=0$ Hartree energy lies quite below the exact ground state and the RPA energy corrections for low T are now more visible. The HF approximation leads, in this case, to a rather good energy estimate for $T=0$.

IV. CONCLUSION

We have shown that within the SPA, the integrals over the static repulsive variables can be accurately evaluated for not too low temperatures in the stationary-phase approximation, around the unique real Hartree solution obtained for given values of the attractive static variables. This enables one to treat the remaining quantal fluctuations also in the Gaussian approximation, above a certain breakdown temperature $T'_c<T_c$. The ensuing CSPA treatment, with the static integrals restricted to the attractive terms, continues to provide a very accurate description of static observables for $T>T'_c$, while the SPA remains quite reliable for $T>T_c$. The present scheme indicates, for instance, how to implement rigorously the CSPA within the pairing plus quadrupole plus dipole model.

At the SPA level, repulsive terms lead to a decrease in the partition function, but their influence on the normalized thermodynamic distribution is negligible beyond the Hartree contribution. More important effects arise at the RPA level for $T<T_c$, where repulsive terms may lead to an enhancement of tunneling effects between the symmetry-breaking mean-field solutions, as seen in the Lipkin model, which are correctly described by the CSPA for $T>T'_c$. In this case configurations away from the stable mean field become relevant in the CSPA also at low temperatures.

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APPENDIX A

The Hamiltonian (1) can be written as

$$H=H(x)-\frac{1}{2}\sum_{\nu} v_{\nu}\left(Q_{\nu}-\frac{x_{\nu}}{v_{\nu}}\right)^{2},$$

$$H(x)=H_0+\sum_{\nu}\frac{x_{\nu}^2}{2v_{\nu}}-x_{\nu}Q_{\nu}. \tag{A1}$$

In the pure attractive case where all $v_{\nu}>0$ (and Q_{ν} is Hermitian), $H(x)-H$ is positive definite for real x and $[H'\equiv H-\mu N,\, H'(x)\equiv H(x)-\mu N]$

$$\mathrm{Tr}\,\exp[-\beta H']\geqslant \mathrm{Tr}\,\exp[-\beta H'(x)] \quad (v_{\nu}>0), \tag{A2}$$

so that $\mathcal{F}\leqslant\mathcal{F}(x)$. In the repulsive case where all $v_{\nu}<0$, $H-H(x)$ is positive definite and

$$\mathrm{Tr}\,\exp[-\beta H']\leqslant \mathrm{Tr}\,\exp[-\beta H'(x)] \quad (v_{\nu}<0), \tag{A3}$$

implying $\mathcal{F}\geqslant\mathcal{F}(x)$. The maximum and minimum value of the right-hand side in Eqs. (A2) and (A3), respectively, is obtained when x is the self-consistent Hartree solution $x_{\nu}=v_{\nu}\langle Q_{\nu}\rangle_x$. The Hartree grand potential $\mathcal{F}_H=\mathcal{F}(x_H)$ is then an upper (lower) bound to $\mathcal{F}$ in the attractive (repulsive) case. If $[H(x),N]=0$, these inequalities hold also in a canonical ensemble, in which case the Hartree average energy

$$E_H=\langle H_0\rangle_{x_H}-\frac{1}{2}\sum_{\nu} v_{\nu}\langle Q_{\nu}\rangle_{x_H}^2$$

provides, for $T\rightarrow 0$, an upper (lower) bound to the ground-state energy in the pure attractive (repulsive) case. If both types of terms are present there is no rule.

On the other hand, the finite-temperature HF partition function follows from a variational principle and always fulfills

$$Z_{\mathrm{HF}}\equiv \mathrm{Tr}\,\exp[-\beta(\langle H'-H'_{\mathrm{HF}}\rangle_{\mathrm{HF}}+H'_{\mathrm{HF}})]\leqslant \mathrm{Tr}\,\exp[-\beta H'], \tag{A4}$$

i.e., $\mathcal{F}_{\mathrm{HF}}\geqslant\mathcal{F}$, where H'_{HF} is the self-consistent operator

$$H'_{\mathrm{HF}}=\sum_{\alpha}\frac{\partial\langle H'\rangle_{\mathrm{HF}}}{\partial\langle P_{\alpha}\rangle_{\mathrm{HF}}}P_{\alpha},$$

with $\{P_{\alpha}\}=\{c_i^{\dagger}c_j\}$ a complete or reduced set of one-body operators. Since $\langle Q_{\nu}^2\rangle_{\mathrm{HF}}\geqslant\langle Q_{\nu}\rangle_{\mathrm{HF}}^2$, the exchange contributions to the average energy included in HF are negative (positive) in the pure attractive (repulsive) case, implying $\mathcal{F}_{\mathrm{HF}}\leqslant\mathcal{F}_H$ ($\mathcal{F}_{\mathrm{HF}}\geqslant\mathcal{F}_H$).

APPENDIX B

In the two-level model, many-body states can be classified into multiplets of definite quasispin J, whose multiplicities $Y(J)$, $0\leqslant J\leqslant\Omega/2$, depend on the ensemble considered [25]. In canonical ensembles, for $N=\Omega$ fermions,

$$Y(J)=\binom{\Omega}{\Omega/2-J}^{\alpha}-\binom{\Omega}{\Omega/2-J-1}^{\alpha}, \tag{B1}$$

where $\alpha=1$ in the restricted SU(2) canonical ensemble of 2^{Ω} many-body states (only one particle for each p is allowed) and $\alpha=2$ in the full canonical ensemble of $\binom{2\Omega}{\Omega}$ many-body states. In the GC ensemble ($2^{2\Omega}$ states)

$$Y(J)=\binom{2\Omega}{\Omega-2J}-\binom{2\Omega}{\Omega-2J-2}. \tag{B2}$$

In this case half integer values of J are also included. The exact partition function for a quasispin Hamiltonian reads then

$$\mathrm{Tr}\,\exp(-\beta H)=\sum_{J=0}^{\Omega/2} Y(J)\sum_{M=-J}^{J} e^{-\beta E_{JM}}, \tag{B3}$$

where E_{JM} are the exact energies (we assumed $N=\Omega$, in which case $\mu=0$ in the GC ensemble). For $H=\boldsymbol{\lambda}\cdot\boldsymbol{J}$, Eq. (B3) becomes

$$\mathrm{Tr}\,\exp(-\beta\boldsymbol{\lambda}\cdot\boldsymbol{J})=\sum_{J} Y(J)\frac{\sinh\beta\lambda(J+\frac{1}{2})}{\sinh\frac{1}{2}\beta\lambda}, \tag{B4}$$

where $\lambda=\sqrt{\boldsymbol{\lambda}\cdot\boldsymbol{\lambda}}$. Equation (B4) holds also for complex $\boldsymbol{\lambda}$. In the GC ensemble, Eq. (B4) can be factorized as

$$\mathrm{Tr}\,\exp(-\beta\boldsymbol{\lambda}\cdot\boldsymbol{J})=[(1+e^{\beta\lambda/2})(1+e^{-\beta\lambda/2})]^{\Omega}, \tag{B5}$$

whereas in the SU(2) canonical ensemble,

$$\mathrm{Tr}\,\exp(-\beta\boldsymbol{\lambda}\cdot\boldsymbol{J})=(e^{\beta\lambda/2}+e^{-\beta\lambda/2})^{\Omega}. \tag{B6}$$

Equations (B5) and (B6) lead then to Eq. (18). The mean-field dynamics is nevertheless the same in these ensembles. The ensemble affects the value of critical temperatures, but not the type of Hartree solutions and transitions.

Denoting now with $|p\nu\rangle$ the single-particle eigenstates of $\boldsymbol{\lambda}\cdot\boldsymbol{J}$, we obtain, setting $\gamma=1/4$ in the GC ensemble and $\gamma=1/2$ in the SU(2) canonical ensemble,

$$\sum_{p,\nu,p',\nu'}\frac{\langle p\nu|J_i|p'\nu'\rangle\langle p'\nu'|J_j|p\nu\rangle(f_{\nu}-f_{\nu'})}{i\omega+\lambda_{\nu'}-\lambda_{\nu}}
=\frac{1}{2}\Omega\frac{\tanh(\beta\gamma\lambda)}{\omega^2+\lambda^2}\left[\lambda\left(\delta_{ij}-\frac{\lambda_i\lambda_j}{\lambda^2}\right)-\omega\varepsilon_{ijk}\frac{\lambda_k}{\lambda}\right], \tag{B7}$$

where $\omega\neq 0$, $\lambda_{\nu}=\nu\lambda/2$, $f_{\nu}=(1+e^{4\gamma\beta\lambda_{\nu}})^{-1}$, $i,j=x,y,z$, and ε_{ijk} is the antisymmetric tensor. We also have

$$\langle\boldsymbol{J}\rangle_{\boldsymbol{\lambda}}\equiv\sum_{p,\nu}\langle p\nu|\boldsymbol{J}|p\nu\rangle f_{\nu}=-\tfrac{1}{2}\Omega\,\tanh[\beta\gamma\lambda]\frac{\boldsymbol{\lambda}}{\lambda},$$

$$-\frac{\partial\langle J_i\rangle_{\boldsymbol{\lambda}}}{\partial\lambda_j}\equiv\sum_{p,\nu,p',\nu'}\langle p\nu|J_i|p'\nu'\rangle\langle p'\nu'|J_j|p\nu\rangle F_{\nu\nu'} \tag{B8}$$

$$=\frac{1}{2}\Omega\left[\frac{\tanh(\beta\gamma\lambda)}{\lambda}\left(\delta_{ij}-\frac{\lambda_i\lambda_j}{\lambda^2}\right)+\frac{\beta\gamma}{\cosh^2(\beta\gamma\lambda)}\frac{\lambda_i\lambda_j}{\lambda^2}\right], \tag{B9}$$

where $F_{\nu\nu'}=(f_\nu-f_{\nu'})/(\lambda_{\nu'}-\lambda_\nu)$ $(\nu\neq\nu')$ and $F_{\nu\nu}=4\gamma\beta f_\nu(1-f_\nu)$.

The HF partition function and equations become

$$Z_{\rm HF}=\mathrm{Tr}\,\exp[-\beta(\langle H-\boldsymbol{\lambda}\cdot\boldsymbol{J}\rangle_{\boldsymbol{\lambda}}+\boldsymbol{\lambda}\cdot\boldsymbol{J})],\qquad (B10)$$

$$\boldsymbol{\lambda}=\partial\langle H\rangle_{\boldsymbol{\lambda}}/\partial\langle \boldsymbol{J}\rangle_{\boldsymbol{\lambda}}.\qquad (B11)$$

For the Hamiltonian (16), $\langle H\rangle_{\boldsymbol{\lambda}}$ can be calculated in the GC ensemble with the expression

$$\tfrac{1}{2}\langle J_iJ_j+J_jJ_i\rangle_{\boldsymbol{\lambda}}=\langle J_i\rangle_{\boldsymbol{\lambda}}\langle J_j\rangle_{\boldsymbol{\lambda}}(1-1/\Omega)+\delta_{ij}\Omega\times(\tfrac{1}{2}\langle \boldsymbol{J}\rangle_{\boldsymbol{\lambda}}^2/\Omega^2+\tfrac{1}{8}),\qquad (B12)$$

where $\langle \boldsymbol{J}\rangle^2=\langle \boldsymbol{J}\rangle\cdot\langle \boldsymbol{J}\rangle$, which follows from Wick's theorem. This no longer holds in canonical ensembles. In the case (B6) we obtain instead

$$\tfrac{1}{2}\langle J_iJ_j+J_jJ_i\rangle_{\boldsymbol{\lambda}}=\langle J_i\rangle_{\boldsymbol{\lambda}}\langle J_j\rangle_{\boldsymbol{\lambda}}(1-1/\Omega)+\tfrac{1}{4}\delta_{ij}\Omega.\qquad (B13)$$

In the Hartree approximation, only the direct term $\langle J_i\rangle\langle J_j\rangle$, of order Ω^2, is retained. The remaining terms (exchange contributions) are of order Ω.

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