VARIATIONAL PAIR THEORY OF MANY-BOSON SYSTEMS: ORIGINS AND APPLICATION TO TRAPPED ATOMIC BEC

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The 1959 Girardeau-Arnowitt (GA) variational pair theory of many-boson systems, the first Hartree-Fock-Bogoliubov theory of such systems, is briefly reviewed, its place in the Hohenberg-Martin classification of "conserving" versus "gapless" theories is described, and the role of three-particle correlations in cancelling the quasiparticle energy gap of the pure pairing theory is explained. Wentzel's nonzero temperature generalization of the zero-temperature GA theory is briefly described. A generalization of the GA theory to the spatially nonuniform case, for application to recent experimentally produced ultralow temperature trapped atomic Bose condensates, is sketched. A key role is played by the concept of "identical twin" pairing, whose relevance stems from a theorem of Zumino on the canonical form of generalized Bose pairing state vectors. Generalizations to nonzero temperature and to time-dependent nonequilibrium phenomena are suggested.

1 Pairing theories of BEC of spatially uniform Bose gases

Consider first a spatially uniform many-boson system whose second-quantized Hamiltonian, taking units $\hbar = m = 1$, has the form

$$\begin{aligned} \hat{H} &= \hat{T} + \hat{U} \\ \hat{T} &= \sum_k \frac{1}{2} k^2 \hat{N}_k \\ \hat{U} &= \frac{1}{2} V^{-1} \sum_{qkk'} \nu_q \hat{a}^\dagger_{k+q} \hat{a}^\dagger_{k'-q} \hat{a}_{k'} \hat{a}_k \end{aligned} \qquad (1)$$

where $\hat{a}_k$ and $\hat{a}^\dagger_k$ are annihilation and creation operators for bosonic atoms with wave vector k, $\hat{N}_k = \hat{a}^\dagger_k \hat{a}_k$ is the corresponding occupation number operator, and ν_q is the Fourier transform of the interatomic interaction potential, assumed to be spherically symmetric. Periodic boundary conditions with macroscopic periodicity cube volume V are assumed and accordingly total linear momentum is conserved. Various theories differ in how much of the interaction operator $\hat{U}$ is retained and how the retained part is treated. Part can be treated exactly in all cases, the $q = 0$ terms of $\hat{U}$ being

$$\hat{U}_0 = \frac{\nu_0}{2} V^{-1} \sum_{kk'} \hat{a}^\dagger_k \hat{a}^\dagger_{k'} \hat{a}_{k'} \hat{a}_k = \frac{\nu_0}{2} V^{-1} \hat{N}(\hat{N} - 1) = (N-1)\frac{\nu_0 n}{2} \qquad (2)$$

where $\hat{N} = \sum_k \hat{N}_k$ is the total atom number operator, N is its eigenvalue, and $n = N/V$ is the atom number density.

1.1 Bogoliubov theory of weakly interacting Bose gas

The well-known Bogoliubov theory of a weakly-interacting Bose gas[1] is based on two approximations: (a) $[\hat{a}_0, \hat{a}_0^\dagger] = 1 \ll \langle \hat{a}_0^\dagger \hat{a}_0 \rangle = n_0 = fN \gg 1$ where f is the Bose-condensed fraction of atoms. For liquid ^{4}He, $N \sim 10^{23}$ and for trapped condensates, $N > 10^3$. Therefore the commutator is negligible compared with the product and the operators are replaced by c-numbers: $\hat{a}_0 \rightarrow \sqrt{n_0}$ and $\hat{a}_0^\dagger \rightarrow \sqrt{n_0}$. (b) Assume $N - n_0 \ll n_0 \approx N$ ($f \approx 1$) and hence retain only interaction terms with two or more (large) factors of $\sqrt{n_0}$. (These approximations are of doubtful accuracy for trapped condensates; they are dropped in the GA pairing theory described in the following section.) The resultant Bogoliubov Hamiltonian is

$$\hat{H}_B = (N-1)\frac{\nu_0 n}{2} + \sum_{k \neq 0} \left(\frac{k^2}{2} + fn\nu_k \right) \hat{N}_k + \frac{fn}{2} \sum_{k \neq 0} \nu_k (\hat{a}_{-k}\hat{a}_k + \hat{a}_k^\dagger \hat{a}_{-k}^\dagger) \quad (3)$$

where the first term, the same as Eq. (2), represents forward scattering, the second represents condensate-noncondensate plane-wave Hartree-Fock with and without exchange, and the last represents $(k, -k)$ pair excitation from and deexcitation to the condensate. This Hamiltonian can be diagonalized by a linear canonical transformation from atom annihilation and creation operators to canonical Bose quasiparticle annihilation and creation operators $\hat{\xi}_k$, $\hat{\xi}_k^\dagger$:

$$\begin{aligned} \hat{\xi}_k &= (1 - L_k^2)^{-1/2} (\hat{a}_k - L_k \hat{a}_{-k}^\dagger) \\ L_k &= (fn\nu_k)^{-1} \left(\omega_k - \frac{k^2}{2} - fn\nu_k \right) \\ \omega_k &= k\sqrt{fn\nu_k + \frac{k^2}{4}} \end{aligned} \quad (4)$$

where ω_k is the quasiparticle energy and has phonon form $\approx ck$ for small k, with sound speed $\sqrt{fn\nu_0}$. The many-body ground state $|\Phi_0\rangle$ is

$$\begin{aligned} |\Phi_0\rangle &= \text{const.} e^{\hat{F}} |n_0\rangle \\ |n_0\rangle &= (n_0!)^{-1/2} (\hat{a}_0^\dagger)^{n_0} |0\rangle \\ \hat{F} &= \frac{1}{2} \sum_{k \neq 0} L_k \hat{a}_k^\dagger \hat{a}_{-k}^\dagger \end{aligned} \quad (5)$$

representing a state with n_0 atoms in the Bose condensate, with all excited (uncondensed) atoms paired $(k,-k)$. (The exponential operator structure is required by the cluster decomposition theorem, in order to yield a thermodynamically extensive ground state energy and an intensive quasiparticle energy.) n_0 is determined from the condition $n_0 + \sum_{k\neq 0}\langle\Phi_0|\hat{N}_k|\Phi_0\rangle = N$. $|\Phi_0\rangle$ is the *quasiparticle vacuum*:

$$\hat{\xi}_k|\Phi_0\rangle = 0\ ,\ k\neq 0 \tag{6}$$

Excited states have quasiparticles excited from the ground state:

$$\mathrm{const.}\hat{\xi}^{\dagger}_{k_1}\hat{\xi}^{\dagger}_{k_2}\cdots|\Phi_0\rangle \tag{7}$$

1.2 Girardeau-Arnowitt variational pair theory

This theory [2], herein denoted by GA, was the first Hartree-Fock-Bogoliubov (HFB) theory of many-boson systems. It is based on the observation that pairing states like that of Bogoliubov, Eq. (5), have nonzero energy expectation value contributions not only from interaction terms retained in the Bogoliubov Hamiltonian (3), but also from two other types of contributions: (a) Terms representing forward scattering of uncondensed particles with exchange, of operator structure $N_k N_{k'}$ with k and k' both nonzero and arising from $q = k'-k\neq 0$ in $\hat{U}$ of Eq. (1). As a matter of fact, terms of the same operator structure, representing forward scattering without exchange and arising from $q=0$, are already included in the c-number term $(N-1)\nu_0 n/2$ of Eq. (3) and hence omission of the corresponding exchange terms is inconsistent, both types together making up the plane-wave Hartree-Fock contributions. (b) Terms of operator structure $\hat{a}^{\dagger}_k\hat{a}^{\dagger}_{-k}\hat{a}_{-k'}\hat{a}_{k'}$ with both k and k' nonzero, representing pair-pair scattering of uncondensed particles and arising from $k'=-k\neq 0\ ,\ q\neq 0$ in Eq. (1). Adding these to the Bogoliubov terms (but now avoiding the Bogoliubov approximation of replacement of $\hat{a}_0$ and $\hat{a}^{\dagger}_0$ by c-numbers) yields all terms in the total Hamiltonian (1) having nonzero expectation values in ground states of pairing form like (5), defining the pair Hamiltonian

$$\begin{aligned}\hat{H}_P &= (N-1)\frac{\nu_0 n}{2} + \sum_{k\neq 0}\left(\frac{k^2}{2}+\frac{\hat{N}_0}{V}\nu_k\right)\hat{N}_k \\ &+(2V)^{-1}\sum_{k\neq 0}\nu_k[\hat{a}^{\dagger}_{-k}\hat{a}^{\dagger}_k\hat{a}_0^2 + (\hat{a}^{\dagger}_0)^2\hat{a}_k\hat{a}_{-k}] \\ &+(2V)^{-1}\sum_{kk'}\nu_{k-k'}\hat{N}_k\hat{N}_{k'} + (2V)^{-1}\sum_{kk'}\nu_{k-k'}\hat{a}^{\dagger}_k\hat{a}^{\dagger}_{-k}\hat{a}_{-k'}\hat{a}_{k'}\end{aligned} \tag{8}$$

where the third summation excludes $k = 0$, $k' = 0$, and $k = \pm k'$ and the last excludes $k = 0$, $k' = 0$, and $k = k'$, in order to avoid double counting. The first two lines are equivalent to the Bogoliubov Hamiltonian except that $\hat{a}_0$ and $\hat{a}_0^\dagger$ are not approximated by c-numbers and the condensate density n_0 is not approximated by the total density n.

The ground state energy and quasiparticle spectrum of this pair Hamiltonian are determined using a variational trial state which is an *exact number eigenstate*, by first defining "quasiunitary" condensate annihilation and creation operators $\hat{\beta}_0 = \hat{a}_0 \hat{N}_0^{-1/2} = e^{i\Theta_0}$ and $\hat{\beta}_0^\dagger = \hat{a}_0^\dagger \hat{N}_0^{-1/2} = e^{-i\Theta_0}$. If the subspace with condensate *totally* depleted ($n_0 = 0$) is neglected then this operator is unitary, the condensate phase operator Θ_0 is hermitian, and for $k \neq 0$

$$[\hat{\beta}_0, \hat{\beta}_0^\dagger] = [\hat{\beta}_0, \hat{a}_k] = [\hat{\beta}_0, \hat{a}_k^\dagger] = 0 \ , \ [\hat{\beta}_0, \hat{N}_0] = \hat{\beta}_0 \tag{9}$$

[Deletion of the $n_0 = 0$ subspace is innocuous so long as the mean condensate occupation $\langle \hat{N}_0 \rangle$ is much greater than the r.m.s. occupation fluctuation. It was shown [2] that for the GA pairing ground state (see below) the condensate fluctuation is normal (of order of the square root of the mean), so this condition is very well satisfied both for macroscopic condensates and trapped atomic condensates, except very near the condensation temperature.] The variational calculation uses a *number conserving* trial ground state of form

$$\begin{aligned} |\Phi_0\rangle &= \text{const.} e^{\hat{F}} |N\rangle = \hat{U} |N\rangle \\ |N\rangle &= (N!)^{-1/2} (\hat{a}_0^\dagger)^N |0\rangle \\ \hat{F} &= \frac{1}{2} \sum_{k\neq 0} \phi_k \hat{a}_k^\dagger \hat{a}_{-k}^\dagger \hat{\beta}_0^2 \\ \hat{U} &= e^{\hat{G}} \ , \ \hat{G} = \frac{1}{2} \sum_{k\neq 0} [\hat{a}_k^\dagger \hat{a}_{-k}^\dagger \hat{\beta}_0^2 - (\hat{\beta}_0^\dagger)^2 \hat{a}_{-k} \hat{a}_k] \tanh^{-1} \phi_k \end{aligned} \tag{10}$$

where ϕ_k is a real, even variational trial function determined by minimization of the variational ground state energy

$$E_0 = \langle \Phi_0 | \hat{H} | \Phi_0 \rangle = \langle \Phi_0 | \hat{H}_P | \Phi_0 \rangle = \langle N | \hat{U}^{-1} \hat{H}_P \hat{U} | N \rangle \ . \tag{11}$$

$|\Phi_0\rangle$ is the vacuum of *number conserving* quasiparticle annihilation operators

$$\hat{\xi}_k = \hat{\beta}_0^\dagger \hat{U} \hat{a}_k \hat{U}^{-1} = (1 - \phi_k^2)^{-1/2} (\hat{\beta}_0^\dagger \hat{a}_k - \phi_k \hat{a}_{-k}^\dagger \hat{\beta}_0) \tag{12}$$

An almost identical number-conserving quasiparticle formalism has been given recently by Gardiner [3] for application to trapped atomic Bose condensates, but makes unnecessary approximations (replacement of n_0 by n) not made in the original GA number-conserving formalism[2]. The relationship between the original GA formalism and that of Gardiner is discussed in a recent Comment[4]. Determination of the ground state and quasiparticle energies involves numerical solution of a nonlinear integral equation which is essentially the Bose version of the BCS energy gap equation. This gives a more accurate ground state energy than that of the Bogoliubov theory, but the quasiparticle energy then has an unwanted energy gap ω_0 given by[2]

$$\omega_0 = 2n_0\nu_0\sqrt{I_0/n_0 v_0} \tag{13}$$

where

$$I_0 = V^{-1}\sum_{k\neq 0}\nu_k\left(\frac{\phi_k}{1-\phi_k^2}\right) = (2\pi)^{-3}\int \nu_k\left(\frac{\phi_k}{1-\phi_k^2}\right)d^3k \tag{14}$$

and ϕ_k is the pairing amplitude occurring in the trial state (10) and the Bogoliubov transformation (12). (The thermodynamic limit $N \to \infty$, $V \to \infty$, $n = N/V$ constant has been taken to convert the sum to an integral.) A nonzero gap violates theorems of Hugenholtz and Pines[5] and Gavoret and Nozières[6]. *This is the price one pays for a more accurate ground state.* The correctness of the GA ground state and quasiparticle spectrum and the above expression for the energy gap *within the framework of pure pairing states* was verified by several independent calculations (Wentzel[7], Takano[8], Hohenberg and Martin[9]). In fact, *three-body correlations* omitted from all pure pairing theories are important near $k = 0$ and can cancel the quasiparticle energy gap. This situation is discussed in the following two subsections.

It is not neccessary to go beyond the GA pair theory to calculate a correct phonon spectrum, if one starts from the fundamental definition of the collective phonon spectrum in terms of the density autocorrelation function. In fact, it was shown by Hohenberg and Martin[9] that the GA theory yields a gapless and more accurate phonon spectrum by such a calculation than is given by the "gapless" Bogoliubov theory. More generally, spectra of other collective excitations (for example, those labelled by angular momentum quantum numbers as in recent experiments on trapped condensates) can be determined from the poles of the Laplace transforms of the persistence amplitudes of the relevant excitations, yielding both energies and damping. (The Bogoliubov theory omits damping effects.)

1.3 Hohenberg-Martin classification: Quasiparticle and collective spectra, gapless vs. conserving theories

Starting from the Schwinger Green's function approach to equilibrium and weakly nonequilibrium statistical mechanics, Hohenberg and Martin [9] classified theories of Bose condensates into two groups: (a) *Conserving* theories: These satisfy hydrodynamic conservation laws implying (among other things) the standard thermodynamic expression for the speed of sound in terms of the compressibility of the ground state. (b) *Gapless* theories: These have a quasiparticle energy which vanishes as $k \rightarrow 0$ (gapless quasiparticle spectrum). They showed that *the GA theory is conserving but not gapless*, whereas *the Bogoliubov theory is gapless but not conserving.* This unpalatable dichotomy has plagued many-boson theory for almost forty years and now presents a problem for theories to support the exciting recent experimental production and investigation of trapped atomic vapor Bose condensates. Such theories should be *both* conserving and gapless for physical consistency. (Although the quasiparticle spectrum is purely discrete for a finite system such as a trapped condensate, even these tiny condensates are large enough that the quasiparticle spectrum is "almost continuous" at low energies, so the distinction between gapless and conserving theories remains relevant.) Motivated by the need for consistent theories of trapped atomic vapor Bose condensates, Griffin has recently [10] revisited the conserving *vs.* gapless dichotomy and controversies.

There is a possible "escape hatch" from this dichotomy which appears to have been overlooked up to now, in that the nonlinear integral equation [2] determining ϕ_k might possess gapless solutions for suitable special forms of effective interaction ν_k. Indeed, it is clear from the expression (14) that the integral I_0 can vanish if ν_k can take on both positive and negative values for suitable ranges of k, in which case the energy gap ω_0 of Eq. (13) would vanish along with I_0. The only explicit expression known for the energy gap is an approximate one obtained [11] by iteration starting with the Bogoliubov approximation, and this iterative procedure is invalid unless $k_0 a \ll 1$ where $\nu_0 = 4\pi a$ (with a the S-wave scattering length) and k_0 is the range of nu_k. Current theories of BEC of trapped atomic vapors almost all use a one-parameter effective potential $\nu_k = 4\pi a =$ const. (Fermi pseudopotential) and this is too crude for investigation of this question, which deserves further study. If gapless solutions of the GA pairing theory (hence of later HFB theories) exist for suitable effective interactions, then the corresponding theories would be *both* conserving and gapless. In contrast, the Popov approximation [12] to HFB theory, currently popular in theories of BEC of trapped atomic vapors, is gapless but not conserving, as is the original Bogoliubov theory [1].

1.4 Three-particle correlations and gapless quasiparticle spectrum

Regardless of whether or not any gapless and conserving solutions of pure pairing theory exist, addition of three-particle correlation terms produces a gapless theory. The relevant interaction terms are those terms of the full interaction $\hat{U}$ of Eq. (1) representing scattering processes in which two excited (noncondensate) particles collide with one falling into the zero-momentum condensate, and the inverse process in which one condensate particle is excited out of the condensate through collision with a noncondensate particle. These define the "triplet" interaction terms

$$\hat{U}_T = V^{-1} \sum_{k k'} \nu_{k-k'} (\hat{a}^{\dagger}_{k-k'} \hat{a}^{\dagger}_{k'} \hat{a}_k \hat{a}_0 + \hat{a}^{\dagger}_0 \hat{a}^{\dagger}_k \hat{a}_{k'} \hat{a}_{k-k'}) \tag{15}$$

where the sum excludes $k = 0$, $k' = 0$, and $k = k'$. Following an initial perturbative estimate [11] indicating that triplet contributions to the quasiparticle energy are of the right order of magnitude to cancel the pairing energy gap (13), it was shown by Takano [8] using a linearized equation of motion method that this energy gap is indeed cancelled by inclusion of $\hat{U}_T$, resulting in a quasiparticle energy of linear phonon form at low k.

Although we are considering here only zero temperature (ground state and low excitations), the triplet contributions also play a crucial role in initial formation of trapped atomic vapor Bose condensates, since the only energy and momentum conserving two-particle collisions of noncondensed (nonzero energy and momentum) particles are those in which two particles of equal momentum magnitude $|k|$ collide at right angles, with one falling into the zero-momentum condensate and the other emerging with momentum magnitude $|k|\sqrt{2}$ in a direction bisecting those of the incident particles. Although the energy eigenstates in a trapping potential are not momentum eigenstates, it remains true that the condensed particles have energies very low compared to the mean energies of uncondensed particles, implying a narrow momentum distribution about $k = 0$. Thus this argument retains qualitative validity, indicating that triplet collision processes, in which two excited atoms collide with one falling into the condensate, play a crucial role in initial formation of the condensate.

1.5 Wentzel's generalization of GA theory to nonzero temperature

The zero-Temperature GA theory was generalized to nonzero temperature by Wentzel [7], using a method [13] of treatment of BCS-like models which yields the exact (in the thermodynamic limit) free energy of the pair Hamiltonian (8). This method is a variant of the Bogoliubov variational principle for the

Helmholtz free energy and is described in detail elsewhere [14]. Wentzel verified the GA expressions [2] for the zero-temperature quasiparticle spectrum and energy gap and generalized to temperature-dependent quasiparticles and free energy.

2 Pairing theories of BEC of trapped atomic vapors at $T = 0$

The many-atom Hamiltonian for bosonic atoms in a trap is

$$\hat{H} = \sum_{nm} (n|H|m)\hat{a}_n^\dagger \hat{a}_m + \frac{1}{2} \sum_{nmlk} (nm|H|lk)\hat{a}_n^\dagger \hat{a}_m^\dagger \hat{a}_k \hat{a}_l \tag{16}$$

where $\hat{a}_n$ and $\hat{a}_n^\dagger$ are annihilation and creation operators for atoms occupying orthonormal basis orbitals $u_n(r)$ to be determined by a self-consistent variational procedure and the matrix elements, in an obvious notation, are

$$\begin{aligned}(n|H|m) &= \int u_n^*(r) \left[-\frac{1}{2}\nabla^2 + v_{\text{trap}}(r) \right] u_m(r) d^3r \\ (nm|H|lk) &= \int u_n^*(r) u_m^*(r') v_{\text{int}}(r - r') u_l(r) u_k(r') d^3r d^3r'\end{aligned} \tag{17}$$

2.1 Generalized pairing

To treat Bose-Einstein condensation in a trap, the $(k, -k)$ pairing of spatially uniform systems has to be generalized. The most general form of pairing involves excitation of pairs of particles to arbitrary excited (uncondensed) states (n, m), by repeated application of pair excitation operators $\hat{a}_n^\dagger \hat{a}_m^\dagger \hat{a}_0^2$ to the completely condensed N-particle state $|N\rangle = (N!)^{-1/2}(\hat{a}_0^\dagger)^N|0\rangle$. Most such theories make the Bogoliubov approximation $\hat{a}_0 \to \sqrt{n_0}$ and $\hat{a}_0^\dagger \to \sqrt{n_0}$. This is questionable for trapped vapors, particularly near the condensation temperature. To avoid this problem one can use the number-conserving formulation of Sec. *1.2*, as in the original GA theory. Then the generalized pairing state is

$$\begin{aligned}|\Phi_0\rangle &= \text{const.} e^{\hat{F}}|N\rangle \\ \hat{F} &= \frac{1}{2} \sum_{nm} g_{nm} \hat{a}_n^\dagger \hat{a}_m^\dagger \hat{\beta}_0^2\end{aligned} \tag{18}$$

generalizing that of Eq. (10), where the sum excludes $n = 0$ and $m = 0$. Since $\hat{a}_n^\dagger$ and $\hat{a}_m^\dagger$ commute, the matrix g_{nm} may be assumed symmetric.

2.2 *Canonical "identical twin" pairing and generalization of GA theory to spatially nonuniform condensates*

Under a unitary transformation of basis $\{u_n\}$ in the subspace orthogonal to the condensate orbital u_0 and a corresponding transformation of the $\hat{a}_n$ and $\hat{a}_n^\dagger$, g_{nm} transforms as a second-rank tensor:

$$g_{nm} \rightarrow \sum_{kl} M_{nk} M_{ml} g_{kl} \tag{19}$$

where M_{nm} is unitary. Zumino's theorem [15] on the canonical form of such a symmetric tensor implies that *there exists a basis* $\{u_n\}$ *in which* g_{nm} *is diagonal, real, and nonnegative.* In such a basis the pairing ground state vector simplifies greatly:

$$|\Phi_0\rangle = \text{const.} e^{\hat{F}} |N\rangle \ , \ \hat{F} = \frac{1}{2} \sum_{n \neq 0} g_n (\hat{a}_n^\dagger)^2 \hat{\beta}_0^2 \tag{20}$$

where g_n is real and nonnegative. One can call this "identical twin pairing". Applicability of Zumino's theorem to simplification of pairing theories of BEC appears to have been overlooked up to now. It is likely to be useful in theories of BEC of trapped atomic vapors, particularly in the case of anisotropic trapping potentials (see following paragraph).

In the case of a spatially uniform system (no trapping potential), theories of many-boson systems almost always use plane-wave orbitals $u_k(r) = V^{-1/2} e^{ik \cdot r}$, and corresponding annihilation operators $\hat{b}_k$. Since the interatomic interaction conserves total linear momentum. the corresponding pair excitation operators are then $\hat{b}_k^\dagger \hat{b}_{-k}^\dagger (\hat{a}_0)^2$. How are these related to canonical Zumino "identical twin" pairing? Define new Bose operators $\hat{a}_k = 2^{-1/2}(\hat{b}_k \pm \hat{b}_{-k})$ where the upper sign is taken for half of k-space (say, the half for which $k_z > 0$) and the lower sign for the other half. Then

$$\hat{b}_k^\dagger \hat{b}_{-k}^\dagger = \frac{1}{2}[(\hat{a}_k^\dagger)^2 + (\hat{a}_{-k}^\dagger)^2] \tag{21}$$

corresponding to Zumino "identical twin" pairing in standing-wave orbitals $(2/V)^{1/2} \cos(k \cdot r)$ and $(2/V)^{1/2} \sin(k \cdot r)$. Conversely, if running-wave orbitals are desired as for axial angular momentum eigenstates with $m \neq 0$ in an axially symmetric trap, then one can transform from canonical $(\hat{a}_n^\dagger)^2$ pairing to angular momentum $(m, -m)$ pairing $\hat{a}_{n,m}^\dagger \hat{a}_{n,-m}^\dagger$, the representation usually used in theories of BEC of atomic vapors in an axially symmetric trap. *Note that this requires a special symmetry property of the trap potential, whereas canonical "identical twin" pairing is completely general.*

In order to generalize the GA variational theory [2] to spatially nonuniform condensates, one determines the amplitude g_n for identical twin pairing in Eq. (20) from the necessary condition $\partial E_0/\partial g_k = 0$ for a minimum of the variational ground state energy E_0. The state (20) is the vacuum of number-conserving quasiparticle operators

$$\hat{\xi}_n = (1 - g_n^2)^{-1/2}(\hat{\beta}_0^\dagger \hat{a}_n - g_n \hat{a}_n^\dagger \hat{\beta}_0) \ , \ n \neq 0 \tag{22}$$

One can show that $|\Phi_0\rangle = \hat{U}|N\rangle$ where

$$\hat{U} = e^{\hat{G}} \ , \ \hat{G} = \frac{1}{2}\sum_{n\neq 0}[(\hat{a}_n^\dagger)^2\hat{\beta}_0^2 - (\hat{\beta}_0^\dagger)^2(\hat{a}_n)^2]\tanh^{-1} g_n \ . \tag{23}$$

The variational ground state energy is

$$E_0 = \langle\Phi_0|\hat{H}|\Phi_0\rangle = \langle N|\hat{U}^{-1}\hat{H}\hat{U}|N\rangle = \langle N|\hat{U}^{-1}\hat{H}_P\hat{U}|N\rangle \tag{24}$$

where $\hat{H}_P$ involves interactions of canonical "identical twin" pairs. Calculations are in progress.

3 Time-dependent pairing theory of trapped condensates

This is a time-dependent canonical Zumino pairing theory motivated by observations of time-dependent phenomena such as the oscillatory coherent tunneling between the two sides of a double-well trap. It is based on the Balian-Vénéroni variational principle for time-dependent nonequilibrium statistical mechanics [16], which stationarizes a *variational trial action*

$$S = i\int_{t_i}^{t} \mathrm{Tr}\{\hat{A}_V(t')\left[i\frac{d}{dt'} - \hat{L}(t')\right]\hat{\rho}_V(t')\}dt' + \mathrm{Tr}[\hat{A}_V(t)\hat{\rho}_V(t)] \tag{25}$$

where $\hat{A}_V(t)$ is a trial operator function for some particular observable $\hat{A}$ whose statistical average is desired at time t, $\hat{\rho}_V(t)$ is a trial statistical density operator, $\hat{L}(t)$ is the Liouville superoperator $\hat{L}(t)\hat{O} = [\hat{H}(t), \hat{O}]$, and $\hat{H}$ is the Hamiltonian. Setting $\delta S = 0$ under unrestricted variations of $\hat{A}_V$ and $\hat{\rho}_V$ with initial constraint $\hat{\rho}_V(t_i) = \hat{\rho}_i$ (initial density operator) and final constraint $\hat{A}_V(t) = \hat{A}$ yields the standard Liouville-von Neumann evolution equation for the statistical density operator (now denoted by $\hat{\rho}_V$) in the Schrödinger picture, together with a *backward* Heisenberg equation for $\hat{A}_V(t)$. By using restricted trial forms for $\hat{A}_V$ and $\hat{\rho}_V$ parameterized by time-dependent functions of t one obtains a "time-dependent Rayleigh-Ritz" calculational method yielding coupled first-order differential equations for these trial functions which can be solved numerically to generate the desired time-dependent statistical average $\langle A(t)\rangle$. One variational parameterization consists of choosing $\hat{\rho}_V(t) = \text{const.}e^{-\beta \hat{H}_{quas}(T,t)}$ with

$$\hat{H}_{quas}(T,t) = \sum_{n\neq 0} \omega_n(T,t)\hat{\xi}_n^\dagger \hat{\xi}_n \tag{26}$$

where the $\hat{\xi}_n$ are the number-conserving quasiparticle operators of Eq. (22) but now with temperature and time-dependent pairing amplitudes $g_n(T,t)$, and $\hat{A}_V$ can likewise be expressed in terms of the same quasiparticle operators, the specific expression being chosen to involve the same operator structures as the quasiparticle representation of the specified observable $\hat{A}$, but now with temperature and time-dependent coefficients. Other parameterizations could also be made and the statistical averages in Eq. (25) would still be calculable in closed form so long as $\hat{\rho}_V$ is taken to be the exponential of a quadratic form in quasiparticle operators. Calculations based on this approach will be described elsewhere.

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