

Conserving *and* gapless approximations for the composite bosons in terms of the constituent fermions

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Abstract. – A well-known problem with the many-body approximations for interacting condensed bosons is the dichotomy between the “conserving” and “gapless” approximations, which either obey the conservation laws or satisfy the Hugenholtz-Pines condition for a gapless excitation spectrum, in the order. It is here shown that such a dichotomy does not exist for a system of *composite bosons*, which form as bound-fermion pairs in the strong-coupling limit of the fermionic attraction. By starting from the constituent fermions, for which conserving approximations can be constructed for any value of the mutual attraction according to the Baym-Kadanoff prescriptions, it is shown that these approximations also result into a gapless excitation spectrum for the boson-like propagators in the broken-symmetry phase.

Many-body descriptions of interacting condensed bosons have long been known [1] to fall into either one of two classes of approximation schemes, which are alternatively consistent with the conservation laws (conserving approximations) or with the absence of a gap in the elementary excitations spectrum (gapless approximations). This constitutes a shortcoming when implementing the many-body theory for condensed bosons, as one would rather like to deal with approximations which are conserving *and* gapless at the same time. This is because the gapless condition ensures the presence of a Goldstone mode [2] associated with the spontaneously broken gauge symmetry; the conserving condition, on the other hand, is required for a proper description of the dynamics of the system.

These approximation schemes have been conceived for systems like helium, for which the internal fermionic structure is immaterial, due to the large energy required to excite the internal fermionic degrees of freedom compared with the energy scales of the experiments. Recent experimental advances with ultracold trapped Fermi atoms, however, have made it possible to produce systems of *composite bosons* (dimers) whose binding energy is comparable with the energy and temperature involved in the experiments [3]. The Bose-Einstein condensation of the dimers has also been detected [4]. In these systems, the internal fermionic structure

is definitely relevant, as the binding energy of the dimers can be tuned via a Fano-Feshbach resonance [5].

For these systems, it appears appropriate to construct the dynamical propagators of the condensed composite bosons in terms of the constituent fermions, by following the progressive quenching of the fermionic degrees of freedom as their attraction is increased. For the constituent fermions, conserving approximations can be constructed for any value of the mutual attraction even in the broken-symmetry (superfluid) phase, via the Baym-Kadanoff prescriptions [6, 7] which require the self-consistent solution of the equations for the single- and two-particle Green's functions. In this way, conservation laws can be regarded to be fulfilled not only in terms of the constituent fermions but also in terms of the composite bosons, when the fermionic attraction gets sufficiently strong. This is because, if the number continuity equation is satisfied in terms of the constituent fermions, it is also satisfied when these fermions are grouped into pairs. The question now is whether such conserving approximations could also lead to a gapless excitation spectrum for the composite bosons in the superfluid phase.

The purpose of this letter is to show that a given fermionic conserving approximation also results in a gapless excitation spectrum for the boson-like propagators of the composite bosons. The practical implications of the present approach will be discussed for the specific example of the fermionic self-consistent t-matrix approximation often used in the literature. The case of a homogeneous system will be considered in the following [8].

Our proof is based on the following arguments. The absence of a gap in the excitation spectrum of composite bosons in the superfluid phase is first proved for the exact theory, in terms of the response of the constituent fermions to an external anomalous-pair source. This entails a connection between single- and two-particle fermionic Green's functions via functional derivative with respect to the external source. In the exact fermionic theory, this connection also implies that the kernel of Dyson's equation for the single-particle Green's function is related to the kernel of the Bethe-Salpeter equation for the two-particle Green's function. Approximate fermionic theories, selected to satisfy the conservation laws on the basis of the Baym-Kadanoff prescriptions [6, 7], require at the same time Dyson's and Bethe-Salpeter equations to be satisfied with the corresponding approximate kernels. This connection between the single- and two-particle Green's functions for an approximate fermionic theory will eventually be used to show that the same theory *also* results into a gapless spectrum for the composite bosons.

We begin by generalizing to the composite bosons the theorem of Hugenholtz-Pines for ordinary bosons [9], by following the treatment of ref. [1] in terms of exact propagators (see also refs. [10, 11] where similar derivations connecting single- and two-particle fermionic Green's functions have been reconsidered). For composite bosons, the Hugenholtz-Pines theorem will be shown to follow from the presence of a nonvanishing order parameter in the superfluid phase. To this end, we define the bosonic-like field operator

$$\Psi_B(\mathbf{r}) = \int d\boldsymbol{\rho} \phi(\rho) \psi_{\downarrow}(\mathbf{r} - \boldsymbol{\rho}/2) \psi_{\uparrow}(\mathbf{r} + \boldsymbol{\rho}/2) \quad (1)$$

for any value of the fermionic coupling, where $\psi_{\sigma}(\mathbf{r})$ is a fermionic field operator with spin σ . When the fermionic attraction is sufficiently strong, the (real and normalized) function $\phi(\rho)$ can be taken as the bound solution of the associated two-body problem. The bosonic order parameter $\alpha(\mathbf{r}) = \langle \Psi_B(\mathbf{r}) \rangle_{\eta}$ is defined as the thermal average of the operator (1) within the restricted (η) ensemble of ref. [1], which breaks the symmetry and makes the thermal average to be nonvanishing. To describe the superfluid phase conveniently, we introduce the Nambu representation ($\Psi_1(\mathbf{r}) = \psi_{\uparrow}(\mathbf{r})$, $\Psi_2(\mathbf{r}) = \psi_{\downarrow}^{\dagger}(\mathbf{r})$), which formally maps anomalous averages of the field ψ_{σ} into normal averages of the Nambu field Ψ_{ℓ} with spinor component ℓ . The

thermal average of the operator (1) can then be expressed in terms of the anomalous fermionic single-particle Green's function \mathcal{G}_{12} :

$$\left\langle \Psi_2^\dagger\left(\mathbf{r} - \frac{\boldsymbol{\rho}}{2}\right) \Psi_1\left(\mathbf{r} + \frac{\boldsymbol{\rho}}{2}\right) \right\rangle_\eta = \mathcal{G}_{12}\left(\mathbf{r} + \frac{\boldsymbol{\rho}}{2}, \mathbf{r} - \frac{\boldsymbol{\rho}}{2}; \tau = 0^-\right) \quad (2)$$

with imaginary time τ .

For the following purposes, it is convenient to consider the generalized fermionic single-particle Green's function:

$$\mathcal{G}(1, 1') = -\frac{\langle T_\tau [S \Psi(1) \Psi^\dagger(1')] \rangle}{\langle T_\tau [S] \rangle} \quad (3)$$

with the notation $1 = (\mathbf{r}_1, \tau_1, \ell_1)$. Here, T_τ is the imaginary-time-ordering operator, $\langle \dots \rangle$ is a thermal average taken with the system grand-canonical Hamiltonian $K = H - \mu N$, $\Psi(1) = \exp[K\tau_1] \Psi_{\ell_1}(\mathbf{r}_1) \exp[-K\tau_1]$, and the operator $S = \exp[-\int d11' \Psi^\dagger(1) U(1, 1') \Psi(1')]$ contains the source term

$$U(1, 1') = \begin{pmatrix} U_n(\mathbf{r}_1, \mathbf{r}_{1'}; \tau_1) & U_s(\mathbf{r}_{1'}, \mathbf{r}_1; \tau_1)^* \\ U_s(\mathbf{r}_1, \mathbf{r}_{1'}; \tau_1) & -U_n(\mathbf{r}_1, \mathbf{r}_{1'}; \tau_1) \end{pmatrix} \delta(\tau_1 - \tau_{1'}^+) \quad (4)$$

with a normal (U_n) and a superfluid (U_s) component which depend explicitly on imaginary time. In this way, the elementary excitations spectrum of the system can be probed. (The superfluid component U_s will be allowed to vanish at the end of the calculation.) In the static case (when U does not depend on the imaginary time), the definition (3) coincides with the ordinary definition (like eq. (2)) within the η -ensemble. With the definition (3), the bosonic order parameter reads:

$$\alpha(\mathbf{r}) = \int d\boldsymbol{\rho} \phi(\boldsymbol{\rho}) \mathcal{G}_{12}\left(\mathbf{r} + \frac{\boldsymbol{\rho}}{2}, \tau; \mathbf{r} - \frac{\boldsymbol{\rho}}{2}, \tau^+\right). \quad (5)$$

Suppose that $U_s(\mathbf{r}, \mathbf{r}'; \tau)$ is varied by a small uniform change of phase $\delta\Phi$, such that $\delta U_s(\mathbf{r}, \mathbf{r}'; \tau) \cong i\delta\Phi U_s(\mathbf{r}, \mathbf{r}'; \tau)$. This change can be reabsorbed by a canonical transformation of the fermionic field operators, so that the corresponding change of the order parameter (5) is given by $\delta\alpha(\mathbf{r}) = -i\delta\Phi\alpha(\mathbf{r})$ to the leading order in $\delta\Phi$. The change $\delta\alpha(\mathbf{r})$ can be calculated *alternatively* via the definitions (5) and (3), by performing the functional derivative of (3) with respect to a variation of U_s :

$$\begin{aligned} \delta\alpha(\mathbf{r}) = & - \int d\boldsymbol{\rho} \phi(\boldsymbol{\rho}) \int d\mathbf{r}_2 d\mathbf{r}'_2 \int d\tau_2 \left[L\left(\mathbf{r} + \frac{\boldsymbol{\rho}}{2}, \tau, 1; \mathbf{r}_2, \tau_2, 2; \mathbf{r} - \frac{\boldsymbol{\rho}}{2}, \tau^+, 2; \mathbf{r}'_2, \tau_2^+, 1\right) \times \right. \\ & \left. \times \delta U_s(\mathbf{r}_2, \mathbf{r}'_2; \tau_2)^* + L\left(\mathbf{r} + \frac{\boldsymbol{\rho}}{2}, \tau, 1; \mathbf{r}_2, \tau_2, 1; \mathbf{r} - \frac{\boldsymbol{\rho}}{2}, \tau^+, 2; \mathbf{r}'_2, \tau_2^+, 2\right) \delta U_s(\mathbf{r}'_2, \mathbf{r}_2; \tau_2) \right]. \quad (6) \end{aligned}$$

Here, $L(1, 2, 1', 2') = \mathcal{G}_2(1, 2, 1', 2') - \mathcal{G}(1, 1')\mathcal{G}(2, 2')$ is the two-particle correlation function expressed in terms of the generalized fermionic two-particle Green's function

$$\mathcal{G}_2(1, 2, 1', 2') = \frac{\langle T_\tau [S \Psi(1) \Psi(2) \Psi^\dagger(2') \Psi^\dagger(1')] \rangle}{\langle T_\tau [S] \rangle}, \quad (7)$$

and is obtained via the functional derivative $L(1, 2, 1', 2') = -\delta\mathcal{G}(1, 1')/\delta U(2', 2)$.

By a similar token, for the adjoint $\alpha(\mathbf{r})^*$ of $\alpha(\mathbf{r})$ one obtains $\delta\alpha(\mathbf{r})^* = i\delta\Phi\alpha(\mathbf{r})^*$, as well as

$$\begin{aligned} \delta\alpha(\mathbf{r})^* = & - \int d\boldsymbol{\rho} \phi(\boldsymbol{\rho}) \int d\mathbf{r}_2 d\mathbf{r}'_2 \int d\tau_2 \left[L\left(\mathbf{r} - \frac{\boldsymbol{\rho}}{2}, \tau, 2; \mathbf{r}_2, \tau_2, 2; \mathbf{r} + \frac{\boldsymbol{\rho}}{2}, \tau^+, 1; \mathbf{r}'_2, \tau_2^+, 1\right) \times \right. \\ & \left. \times \delta U_s(\mathbf{r}_2, \mathbf{r}'_2; \tau_2)^* + L\left(\mathbf{r} - \frac{\boldsymbol{\rho}}{2}, \tau, 2; \mathbf{r}_2, \tau_2, 1; \mathbf{r} + \frac{\boldsymbol{\rho}}{2}, \tau^+, 1; \mathbf{r}'_2, \tau_2^+, 2\right) \delta U_s(\mathbf{r}'_2, \mathbf{r}_2; \tau_2) \right] \quad (8) \end{aligned}$$

in place of (6). (The quantity $\alpha(\mathbf{r})^*$ is defined like in eq. (5) with \mathcal{G}_{21} replacing \mathcal{G}_{12} .)

The static and uniform limit of the above results can be considered at this point. Without loss of generality, we let $U_s(\mathbf{r}, \mathbf{r}'; \tau) \rightarrow U_s \phi(|\mathbf{r} - \mathbf{r}'|)$ in both eqs. (6) and (8), where U_s is a (complex) constant and ϕ is the function of eq. (1). We also introduce the Fourier representation:

$$L(1, 2, 1', 2') = \int \frac{d\mathbf{p}}{(2\pi)^3} \frac{1}{\beta} \sum_n \int \frac{d\mathbf{p}'}{(2\pi)^3} \frac{1}{\beta} \sum_{n'} \int \frac{d\mathbf{q}}{(2\pi)^3} \frac{1}{\beta} \sum_\nu e^{i(\mathbf{p}+\mathbf{q})\cdot\mathbf{r}_1} e^{i\mathbf{p}'\cdot\mathbf{r}_2} e^{-i\mathbf{p}\cdot\mathbf{r}'_1} e^{-i(\mathbf{p}'+\mathbf{q})\cdot\mathbf{r}'_2} \times \\ \times e^{-i(\omega_n+\Omega_\nu)\tau_1} e^{-i\omega_{n'}\tau_2} e^{i\omega_n\tau'_1} e^{i(\omega_{n'}+\Omega_\nu)\tau'_2} L_{\ell'_1\ell'_2}^{\ell_1\ell_2}(p, p'; q). \quad (9)$$

Here, \mathbf{p} , \mathbf{p}' , and \mathbf{q} are wave vectors, $\omega_n = (2n+1)\pi/\beta$ (n integer) is a fermionic Matsubara frequency (β being the inverse temperature), $\Omega_\nu = 2\pi\nu/\beta$ (ν integer) a bosonic Matsubara frequency, and $p = (\mathbf{p}, \omega_n)$, $p' = (\mathbf{p}', \omega_{n'})$, and $q = (\mathbf{q}, \Omega_\nu)$ are four-vectors. By manipulating eqs. (6) and (8), and by recalling the identities $\delta\alpha(\mathbf{r}) = -i\delta\Phi\alpha(\mathbf{r})$ and $\delta U_s(\mathbf{r}, \mathbf{r}'; \tau) = i\delta\Phi U_s(\mathbf{r}, \mathbf{r}'; \tau)$ (plus their adjoints), one ends up with the matrix equation

$$\begin{pmatrix} \alpha \\ -\alpha \end{pmatrix} = \begin{pmatrix} G_{22}^{11}(q \rightarrow 0) & G_{21}^{12}(q \rightarrow 0) \\ G_{12}^{21}(q \rightarrow 0) & G_{11}^{22}(q \rightarrow 0) \end{pmatrix} \begin{pmatrix} U_s \\ -U_s \end{pmatrix} \quad (10)$$

for U and α real, with the notation

$$G_{\ell'_1\ell'_2}^{\ell_1\ell_2}(q) = - \int \frac{d\mathbf{p}}{(2\pi)^3} \frac{1}{\beta} \sum_n e^{i\omega_n 0^+} \int \frac{d\mathbf{p}'}{(2\pi)^3} \frac{1}{\beta} \sum_{n'} e^{i\omega_{n'} 0^+} \phi(\mathbf{p}+\mathbf{q}/2) \phi(\mathbf{p}'+\mathbf{q}/2) L_{\ell'_1\ell'_2}^{\ell_1\ell_2}(p, p'; q). \quad (11)$$

In the limit $U_s \rightarrow 0$, the definition (11) corresponds to the normal and anomalous bosonic-like propagators, which can be constructed with the operator (1) and its adjoint in the superfluid phase and which embody the elementary excitations spectrum of the system.

Before letting $U_s \rightarrow 0$ in eq. (10), we introduce the inverse of the matrix on its right-hand side and write

$$\begin{pmatrix} G_{22}^{11}(q \rightarrow 0) & G_{21}^{12}(q \rightarrow 0) \\ G_{12}^{21}(q \rightarrow 0) & G_{11}^{22}(q \rightarrow 0) \end{pmatrix} = \frac{1}{AD - BC} \begin{pmatrix} D & -B \\ -C & A \end{pmatrix}. \quad (12)$$

Matrix inversion of eq. (10) then yields the conditions

$$A - B = 0, \quad C - D = 0, \quad (13)$$

in order to have a nonvanishing value for the order parameter α in the limit $U_s \rightarrow 0$. These conditions are not independent of each other, since one can prove from time-reversal invariance that $A = D$ and $B = C$. The denominator in eq. (12) then reduces to $AD - BC = (A - B)(A + B)$, and vanishes owing to (13). The bosonic-like propagators (11) are thus singular when $q \rightarrow 0$, irrespective of the value of the fermionic coupling. This implies, in particular, that the *composite bosons*, which form when the fermionic attraction is strong enough, have a *gapless* spectrum of the elementary excitations. In the present context, the condition $A - B = 0$ thus corresponds to the Hugenholtz-Pines theorem for ordinary bosons.

All considerations made so far hold for the exact fermionic single- (eq. (3)) and two-particle (eq. (7)) Green's functions. The crucial step to derive the result (10) was that these Green's functions are related to each other via a functional differentiation in the presence of the external potential U . To extend the above results to approximate treatments of fermions, it is convenient to explore this relation further [6, 7], by exploiting Dyson's equation:

$$-\mathcal{G}^{-1}(1, 2) = \frac{\partial}{\partial \tau_1} \delta(1, 2) + M(1, 2) + U(1, 2) + \Sigma(1, 2). \quad (14)$$

Here, $M(1, 2) = \tau_{\ell_1 \ell_2}^3 (h(\mathbf{r}_1) - \mu) \delta(\mathbf{r}_1 - \mathbf{r}_2) \delta(\tau_1 - \tau_2)$ where τ^3 is a Pauli matrix and $h(\mathbf{r})$ is the single-particle Hamiltonian, and Σ is the fermionic self-energy. The two-particle correlation function L is correspondingly obtained as

$$\begin{aligned}
 -L(1, 2, 1', 2') &= \frac{\delta \mathcal{G}(1, 1')}{\delta U(2', 2)} = - \int d34 \mathcal{G}(1, 3) \frac{\delta \mathcal{G}^{-1}(3, 4)}{\delta U(2', 2)} \mathcal{G}(4, 1') \\
 &= \mathcal{G}(1, 2') \mathcal{G}(2, 1') + \int d3456 \mathcal{G}(1, 3) \mathcal{G}(6, 1') \frac{\delta \Sigma(3, 6)}{\delta \mathcal{G}(4, 5)} (-) L(4, 2, 5, 2'). \quad (15)
 \end{aligned}$$

It satisfies the Bethe-Salpeter equation, with kernel $\delta \Sigma / \delta \mathcal{G}$ related to the kernel Σ of Dyson's equation. The limit $U \rightarrow 0$ is taken in eqs. (14) and (15) when appropriate.

Selection of an approximate fermionic theory, which preserves the gapless nature of the bosonic-like propagators, proceeds along the following lines. An approximate choice of the functional form of the self-energy Σ in terms of \mathcal{G} (and of the two-body interaction) is made. Equations (14) and (15) are then solved self-consistently, with the respective approximate kernels Σ and $\delta \Sigma / \delta \mathcal{G}$. Equation (15) then implies that eq. (6) (and its adjoint (8)) holds even for the approximate theory, since L (with the approximate kernel $\delta \Sigma / \delta \mathcal{G}$) still represents the functional derivative of \mathcal{G} with respect to U . The alternative result $\delta \alpha(\mathbf{r}) = -i \delta \Phi \alpha(\mathbf{r})$ is instead obtained in the approximate theory by noting that, under the transformation $U_s(\mathbf{r}, \mathbf{r}'; \tau) \rightarrow e^{i \delta \Phi} U_s(\mathbf{r}, \mathbf{r}'; \tau)$, the approximate off-diagonal single-particle Green's function \mathcal{G}_{12} of eq. (5) transforms as $\mathcal{G}_{12} \rightarrow e^{i \delta \Phi} \mathcal{G}_{12}$. As a consequence, the result (13) follows, implying a *gapless* spectrum even for the approximate theory.

Conserving approximations for fermions are similarly based on eqs. (14) and (15), solved self-consistently for an approximate choice of Σ . In this case, however, the self-energy needs to be chosen appropriately, to comply with the requirements of local number conservation and gauge invariance [12]. It is then required that the symmetry property $L(1, 2, 1', 2') = L(2, 1, 2', 1')$ is satisfied by the approximate L . To this end, it is sufficient that the approximate

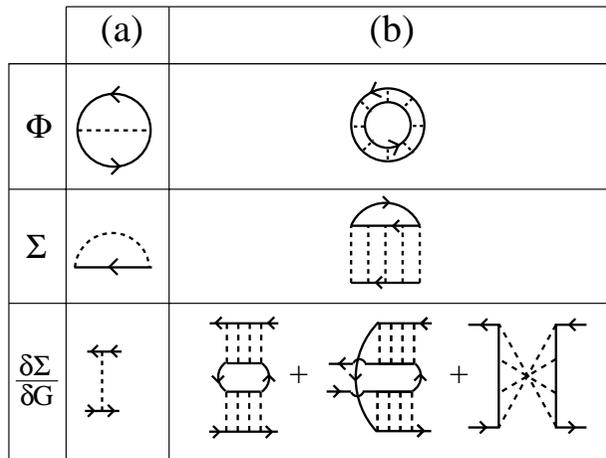


Fig. 1 – Self-energy Σ derived from the potential Φ with the associated kernel $\delta \Sigma / \delta \mathcal{G}$, for (a) the BCS approximation and (b) the t-matrix approximation in the broken-symmetry phase. Full lines represent fermionic (self-consistent) single-particle Green's functions, with the arrows pointing from the second to the first argument; broken lines represent the fermionic interaction potential.

kernel $\delta\Sigma/\delta\mathcal{G}$ of eq. (15) satisfies the same symmetry property. This property is, in turn, met by any Φ -derivable approximation for the self-energy Σ of eq. (14), whereby $\Sigma(1,2) = \delta\Phi/\delta\mathcal{G}(2,1)$ is obtained from an approximate functional Φ [7].

Such fermionic conserving approximations will also result in a gapless spectrum for the composite bosons, as the same requirement for eqs. (14) and (15) to be simultaneously and self-consistently satisfied applies to both (conserving *and* gapless) procedures. This proves our claim, since being conserving for fermions also implies being conserving for composite bosons when fermions are grouped into pairs.

A well-known example of a fermionic conserving approximation, which results for any coupling into a gapless spectrum for the collective mode in the broken symmetry [12], is the BCS approximation for Σ , shown in fig. 1(a) with the potential Φ and the kernel $\delta\Sigma/\delta\mathcal{G}$. In this case, the self-consistent solution of Dyson's equation (14) simply reduces to the solution of the BCS gap equation. This equation, in turn, coincides with the condition $A - B = 0$ of eq. (13) which guarantees the absence of a gap in the bosonic excitation spectrum. In this case, the self-consistent solution of the BCS gap equation is thus sufficient for the approximation to be conserving *and* gapless at the same time. More generally, joint solution of eqs. (14) and (15) is required for the approximation to be conserving and gapless. For instance, to the self-energy Σ within the fermionic t-matrix approximation in the broken-symmetry phase [13] there correspond three distinct contributions to the kernel $\delta\Sigma/\delta\mathcal{G}$ (cf. fig. 1(b)). When considering the BCS and t-matrix approximations for Σ together, to get a gapless spectrum it is thus not enough to solve self-consistently Dyson's equation for \mathcal{G} with both self-energy contributions, if one solved at the same time the Bethe-Salpeter equation with only the BCS contribution to kernel $\delta\Sigma/\delta\mathcal{G}$. By doing so, one would omit the three contributions to $\delta\Sigma/\delta\mathcal{G}$ of fig. 1(b), which are required by conserving criteria. Additional conserving *and* gapless approximations may be similarly constructed by suitable choices of Σ .

It should, finally, be mentioned that a prior attempt was made in ref. [14] to construct an approximation for ordinary bosons which is simultaneously conserving and gapless. This was made within a dielectric formalism by relying on the diluteness condition for the bosons, which makes conservation laws to be satisfied only perturbatively. It could thus be applied to composite bosons only in the extreme strong-coupling limit of the fermionic attraction and not in the intermediate-coupling region of interest.

In conclusion, we have shown that a given conserving approximation for the constituent fermions also results into a gapless spectrum for the composite bosons. Although the self-consistent solution of the equations determining the fermionic single- and two-particle Green's functions might, in general, involve considerable numerical labor, enforcing the fermionic conserving criteria proves *per se* sufficient to get a gapless bosonic spectrum.

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