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TWO-BODY CORRELATIONS IN QUANTUM MANY-BODY SYSTEMS: A CONFRONTATION BETWEEN DIFFERENT TECHNIQUES

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1. INTRODUCTION

The best of the currently available microscopic techniques in *ab initio* quantum many-body theory have been widely applied to many different physical systems, where they have often been found to be capable of high precision in relatively low orders of implementation. Most practitioners nowadays believe that the state of the art in quantum many-body theory is such that it is less important to develop fundamentally new techniques, for which there seems to be no real need, than to explore the relationships between existing methods which are capable of systematic improvement via well-defined hierarchical approximation schemes. Although different such schemes in principle agree when carried out to the highest (usually infinite) order necessary for a complete description of the system under study, they will naturally differ in practice when truncated. In particular, the incorporation of the important, and usually dominant, two-body correlation effects depends critically on the formalism adopted.

The aim of the present paper is to examine in depth the relationships between different methods of building two-body correlations into the many-body wave function in various theoretical frameworks. We are particularly interested in studying fully microscopic approaches, as opposed to the more phenomenological techniques that are not intended or designed for systematic improvement. We therefore focus on the following approaches: (i) the coupled cluster method [1-7]; (ii) variational techniques based on Jastrow-correlated wave functions [8-16]; (iii) planar (or parquet) theory [13,17-22]; and (iv) a nonlinear integro-differential equation approach due to Lieb [23-25].

The comparison is made by applying each technique to a particular model problem for which exact results are known. This is chosen to be the so-called Lieb model [26-30] of an infinite system of bosons constrained to move on the one-dimensional line, at a fixed density, and interacting via a pairwise repulsive delta-function potential. The strong-coupling limit thus corresponds to the case of one-dimensional hard-core bosons. The model is known to be exactly integrable *for all values of the coupling constant* by the Bethe-ansatz technique [30-32]. Like most exactly soluble models, the Lieb model provides an especially stringent test for the universal techniques of quantum many-body theory considered here.

One of our main aims in this work has been to show that by bringing the various theoretical methodologies into confrontation by applying each of them to a specific model, we can gain valuable insight both into the methods themselves and, perhaps even more importantly, into the various interconnections between them. We shall also show how, by bringing into conjunction the best elements of the existing methods described, we might produce powerful new calculational schemes.

The remainder of the paper is organized as follows. The Lieb model and its exact solution are first described in Sec. 2. In Secs. 3-5 we then describe in turn the elements of the coupled cluster method (CCM), the local parquet approximation (LPA), and the nonlinear integro-differential equation approach (NIEA) of Lieb. The CCM is also applied in Sec. 3 to the Lieb model at the so-called SUB2 level of approximation, and corresponding results are given in Secs. 4 and 5 for the LPA and NIEA methods. In the light of the latter results we return in Sec. 6 to consider improved truncation schemes within the CCM framework. We conclude in Sec. 7 with a critical discussion of the results obtained.

2. THE LIEB MODEL OF INTERACTING BOSONS

The so-called Lieb model [26-30] considered here consists of a homogeneous system of N bosons constrained to lie on a line of length L interacting via a repulsive pairwise delta-function potential, $v(x) = 2c\delta(x)$, where $c > 0$ and x is the interparticle spacing. The Hamiltonian for the system, in units in which $\hbar = 2m = 1$, is given by,

$$H = -\sum_{i=1}^{N} \partial^2/\partial x_i^2 + 2c \sum_{1 \le i < j \le N} \delta(x_i - x_j) \ . \tag{2.1}$$

We are particularly interested here in the ground-state Schrödinger equation,

$$H\Psi = E\Psi \ , \tag{2.2}$$

in the thermodynamic limit where $N \to \infty$, $L \to \infty$, such that $\rho \equiv N/L$ remains finite; and with a bosonic solution $\Psi = \Psi(x_1, \cdots, x_n)$ which is symmetric under the interchange of any two coordinates, and which obeys periodic boundary conditions in each coordinate separately.

Lieb and Liniger [26] first showed that Eqs. (2.1) and (2.2) could be solved exactly by a Bethe ansatz [32] form for the wave function. This general technique has now become of great importance as a method of solution for a number of exactly integrable quantum field theory and statistical mechanical models in two space-time dimensions.

All such models solvable by means of the Bethe ansatz share the following feature, namely that they can be reduced to two-body dynamics, in complete analogy with the reduction of free models to one-body dynamics. More precisely, the many-particle scattering matrix simply becomes a product of two-particle scattering matrices, with the latter obeying a particular self-consistency relation. This relation is just the corresponding Yang-Baxter equation (and see Ref. [33]) for the model. The latter equation is nowadays regarded as perhaps the fundamental concept for exactly soluble models. Indeed, the role of the Yang-Baxter equation extends beyond the theory of dynamical systems into both knot theory and the theory of quantum groups. Furthermore, from a modern viewpoint, the coordinate-space Bethe ansatz generalises into an algebraic counterpart and thence into the quantum inverse scattering method which lies at the heart of present treatments of exactly integrable two-dimensional models in quantum field theory and quantum statistical mechanics. The interested reader is referred to Ref. [31] for a modern treatment of the subject, which actually begins with a detailed discussion of the Lieb model, brief details of the solution to which are given below.

Due to the symmetry of Ψ it is sufficient to consider the solution in the domain R where $0 \leq x_1 < x_2 < \cdots < x_N \leq L$. The wave function in R is simply an eigenfunction of the *free* Hamiltonian,

$$-\sum_{i=1}^{N} \partial^2 \Psi / \partial x_i^2 = E\Psi; \quad \text{in } R \ , \tag{2.3}$$

together with the boundary conditions,

$$(\partial/\partial x_{j+1} - \partial/\partial x_j - c)\Psi = 0; \quad x_{j+1} = x_j + 0 \ . \tag{2.4}$$

Equations (2.3) and (2.4) are fully equivalent to Eqs. (2.1) and (2.2). Now, it is readily verified that the (unnormalized) function Ψ specified in R as

$$\Psi = \prod_{1 \leq i < j \leq N} (\partial/\partial x_j - \partial/\partial x_i + c) \det[\exp(ik_m x_n)] \ , \tag{2.5}$$

satisfies Eqs. (2.3) and (2.4) with

$$E = \sum_{i=1}^{N} k_i^2 \ , \tag{2.6}$$

and where the parameters $\{k_i; i = 1, \cdots, N\}$ are any set of distinct numbers. One also observes that Ψ given by Eq. (2.5) is an antisymmetric function of the parameters $\{k_i\}$. Hence $\Psi = 0$ if $k_i = k_j, i \neq j$, and this forms the basis of the set $\{k_i\}$ forming *a filled Fermi (or Dirac) sea*, which appears strange at first sight for a bosonic problem.

Finally, the set $\{k_i\}$ is determined by requiring that $\Psi(x_1, \cdots, x_i, \cdots, x_N) = \Psi(x_1, \cdots, x_i + L, \cdots, x_N)\ \forall i$, or equivalently that $\Psi(0, x_2, \cdots, x_N) = \Psi(x_2, \cdots, x_N, L)$ for Ψ defined in the domain R. These requirements result in the following Bethe equations for the permitted values of $\{k_j\}$,

$$\exp(ik_j L) = -\prod_{l=1}^{N} \frac{k_j - k_l + ic}{k_j - k_l - ic} \ ; \quad j = 1, \cdots, N \ , \tag{2.7}$$

or equivalently,

$$(-1)^{N-1} \exp(-ik_j L) = \exp\left[i \sum_{l=1}^{N} \theta(k_l - k_j) \right] \ ; \quad j = 1, \cdots, N \ , \tag{2.8a}$$

$$\theta(k) \equiv -2\tan^{-1}(k/c)\ ; \quad -\pi < \theta < \pi, \quad k \in \mathbf{R}\ . \tag{2.8b}$$

Although Eqs. (2.7) or (2.8) comprise N equations in N unknowns they have many sets of solutions (corresponding to the different eigenfunctions of the Hamiltonian). Equation (2.8a) may be rewritten as

$$\delta_j \equiv (k_{j+1} - k_j)L = \sum_{i=1}^{N}[\theta(k_i - k_j) - \theta(k_i - k_{j+1})] + 2\pi n_j\ ; \quad j = 1, \cdots, N-1\ , \tag{2.9}$$

where n_j is an integer. Equation (2.9) comprises $(N-1)$ simultaneous equations for the set $\{\delta_j\}$, from the solution to which the set $\{k_j\}$ may be found once k_1 is fixed from Eq. (2.8a). One can show that with all $n_j \geq 1$ there is a solution to Eq. (2.8) with real $\delta_j > 0$.

If we pass now to the bulk thermodynamic limit the ground state will be obtained with all $n_j = 1$, since this clearly minimizes E from Eq. (2.6). In this limit, furthermore, the set $\{k_j\}$ becomes dense over the "Dirac sea" $-K \leq k \leq K$ with a (non-uniform) distribution $f(k)$ such that $Lf(k)dk$ is the number of k parameters in the range $k \to k + dk$. One can then easily show that Eq. (2.9) reduces to the integral equation,

$$1 = -2c\int_{-K}^{K} dk' \frac{f(k')}{c^2 + (k-k')^2} + 2\pi f(k)\ , \tag{2.10a}$$

with the condition that the number of particles is N given by,

$$\int_{-K}^{K} dk\ f(k) = \rho\ , \tag{2.10b}$$

and the ground-state energy given from Eq. (2.6) by,

$$E = L\int_{-K}^{K} dk\ k^2 f(k)\ . \tag{2.10c}$$

It is now convenient to introduce the dimensionless coupling constant,

$$\gamma \equiv c/\rho\ , \tag{2.11}$$

in terms of which the ground-state energy E may be written as,

$$E \equiv N\rho^2 e(\gamma)\ . \tag{2.12}$$

By writing $c \equiv K\lambda, k \equiv Kx, f(Kx) \equiv g(x)$, Eqs. (2.10a-c) become,

$$1 + 2\lambda\int_{-1}^{1} dx' \frac{g(x')}{\lambda^2 + (x-x')^2} = 2\pi g(x)\ , \tag{2.13a}$$

$$\gamma\int_{-1}^{1} dx\ g(x) = \lambda\ , \tag{2.13b}$$

$$e(\gamma) = \left(\frac{\gamma}{\lambda}\right)^3 \int_{-1}^{1} dx\ x^2 g(x)\ . \tag{2.13c}$$

We have solved Eqs. (2.13a-c) numerically. The values are tabulated in Tables 1 and 2 given in later Sections. The method of solution is first to solve Eq. (2.13a) for $g(x)$ for a given value of λ. Equation (2.13b) then determines $\gamma = \gamma(\lambda)$. This process is repeated until the solution for a required value of γ is obtained.

The above exact solutions lead to the following analytic results for e in the small- and large-γ limits,

$$e(\gamma) \underset{\gamma \to 0}{\longrightarrow} \gamma - \frac{4}{3\pi}\gamma^{\frac{3}{2}} \quad , \tag{2.14}$$

$$e(\gamma) \underset{\gamma \to \infty}{\longrightarrow} \frac{\pi^2}{3} \quad . \tag{2.15}$$

We also note an interesting feature of the Lieb model, namely that the integral equation (2.13a) is easy to solve for large c (or γ), but as $c \to 0$ (or $\gamma \to 0$) the solution becomes increasingly singular. This feature seems to be true of all the exactly soluble models, and is the opposite of what one finds from their approximate treatments by the general many-body formalisms discussed below, where the weak-coupling limit is the simplest regime to obtain correctly but the strong-coupling limit is difficult. Finally, we note that, although we do not discuss them further here, the elementary excitations of the Lieb model for all $c > 0$ look like the spectrum of ideal fermions (rather than bosons), for reasons to which we have already alluded.

3. COUPLED CLUSTER METHOD: SUBn APPROXIMATION

The basic coupled cluster method (CCM) approach is by now well known, and we refer the reader to the literature [5-7] for the details of the underlying philosophy and its most general features. Instead, we concentrate here on its specific application to the bosonic systems of interest. We consider a zero-temperature system comprising N bosons in a d-dimensional volume Ω, and we shall mostly be concerned with the thermodynamic limit where $N \to \infty$, $\Omega \to \infty$, such that $\rho \equiv N/\Omega$ remains finite.

The basic boson destruction and creation operators are $b(\mathbf{q})$ and $b^\dagger(\mathbf{q})$ respectively in the momentum-space representation, with the usual canonical commutation relations,

$$[b(\mathbf{q}), b(\mathbf{q}')] = 0 \; ; \quad [b(\mathbf{q}), b^\dagger(\mathbf{q}')] = (2\pi)^d \Omega^{-1} \delta(\mathbf{q} - \mathbf{q}') \quad , \tag{3.1}$$

where $\delta(\mathbf{q})$ is the d-dimensional Dirac delta function. The zero-momentum term is conveniently separated explicitly as,

$$b(\mathbf{q}) = \bar{b}(\mathbf{q}) + \Omega^{-1}(2\pi)^d \delta(\mathbf{q}) b_0 \; ; \quad \bar{b}(q = 0) = 0 \quad . \tag{3.2}$$

Introducing the definition of the Fourier transform of the destruction operator $b(\mathbf{q})$ as,

$$b(\mathbf{x}) = \Omega \int \frac{d\mathbf{q}}{(2\pi)^d} e^{-i\mathbf{q}\cdot\mathbf{x}} b(\mathbf{q}) \Longleftrightarrow b(\mathbf{q}) = \frac{1}{\Omega} \int d\mathbf{x} \; e^{i\mathbf{q}\cdot\mathbf{x}} b(\mathbf{x}) \quad , \tag{3.3}$$

the coordinate-space analogue of the boson destruction operator is,

$$b(\mathbf{x}) = \bar{b}(\mathbf{x}) + b_0 \quad . \tag{3.4}$$

The two-body potential term in the many-body Hamiltonian of Eq. (2.1) may be written quite generally in second-quantized form as,

$$\hat{V} = \frac{1}{2}\frac{1}{\Omega^2} \int d\mathbf{x}_3 \int d\mathbf{x}_4 v(\mathbf{x}_3, \mathbf{x}_4) b^\dagger(\mathbf{x}_3) b^\dagger(\mathbf{x}_4) b(\mathbf{x}_4) b(\mathbf{x}_3)$$

$$\equiv \frac{1}{2} \int \int_{34} v(34) b^\dagger(3) b^\dagger(4) b(4) b(3) \quad , \tag{3.5}$$

where $v(34) \equiv v(\mathbf{x}_3, \mathbf{x}_4) = v(\mathbf{x}_3 - \mathbf{x}_4)$ and $b(i) \equiv b(\mathbf{x}_i)$, and in a notation where,

$$\int \cdots \int_{1 \cdots n} f(1 \cdots n) \equiv \frac{1}{\Omega^n} \int d\mathbf{x}_1 \cdots \int d\mathbf{x}_n \; f(\mathbf{x}_1, \cdots, \mathbf{x}_n) \quad . \tag{3.6}$$

The exact ground-state wave function $|\Psi\rangle$ of the many-body Hamiltonian H is now written in the general CCM form,

$$|\Psi\rangle = e^S |\Phi\rangle \quad , \tag{3.7}$$

in terms of an exponentiated correlation operator S and some suitable model state $|\Phi\rangle$. For bosons we choose $|\Phi\rangle$ to be the normalized zero-momentum condensate,

$$|\Phi\rangle = (N!)^{-\frac{1}{2}} (b_0^\dagger)^N |0\rangle \; ; \quad \langle \Phi | \Phi \rangle = 1 \quad , \tag{3.8}$$

in terms of the bosonic vacuum state $|0\rangle$,

$$b_0 |0\rangle = 0 = \bar{b}(\mathbf{q}) |0\rangle \quad . \tag{3.9}$$

The correlation operator S may be decomposed into its n-body partitions,

$$S = \sum_{n=2}^{N} S_n \quad , \tag{3.10}$$

where S_n may be expressed in the coordinate-space representation as,

$$S_n = \frac{1}{n!} \int \cdots \int_{12 \cdots n} S_n(12 \cdots n) \bar{b}^\dagger(1) \bar{b}^\dagger(2) \cdots \bar{b}^\dagger(n) b_0^n \quad , \tag{3.11}$$

where $S_n(12 \cdots n)$ is a completely symmetric function of its n position coordinates. We note that Eqs. (3.7) and (3.8) imply the intermediate normalization condition for $|\Psi\rangle$,

$$\langle \Phi | \Psi \rangle = \langle \Phi | \Phi \rangle = 1 \quad . \tag{3.12}$$

It is also convenient to define the momentum-space matrix elements of the operator S_n as follows,

$$S_n(\mathbf{q}_1, \cdots, \mathbf{q}_n) \equiv \frac{1}{\Omega} \int d\mathbf{x}_1 \cdots \int d\mathbf{x}_n \; e^{i\mathbf{q}_1 \cdot \mathbf{x}_1} \cdots e^{i\mathbf{q}_n \cdot \mathbf{x}_n} S_n(\mathbf{x}_1, \cdots, \mathbf{x}_n) \quad . \tag{3.13}$$

We note that translational invariance implies that for an arbitrary translational vector $\mathbf{a}$,

$$S_n(\mathbf{x}_1 + \mathbf{a}, \cdots, \mathbf{x}_n + \mathbf{a}) = S_n(\mathbf{x}_1, \cdots, \mathbf{x}_n) \quad , \tag{3.14a}$$

or, equivalently, in momentum-space representation,

$$S_n(\mathbf{q}_1, \cdots, \mathbf{q}_n) = S_n(\mathbf{q}_1, \cdots, \mathbf{q}_n)(2\pi)^d \Omega^{-1} \delta(\mathbf{q}_1 + \cdots + \mathbf{q}_n) \quad . \tag{3.14b}$$

For example, in the case $n = 2$ we have $S_2(\mathbf{x}_1, \mathbf{x}_2) = S_2(\mathbf{x}_1 - \mathbf{x}_2)$; and we also write $S_2(\mathbf{q}, -\mathbf{q}) \equiv S_2(q)$. Finally, we note that translational invariance implies that the one-body partition $S_1 \equiv 0$, as assumed in Eq. (3.10).

By projecting the ground-state Schrödinger equation,

$$H |\Psi\rangle = E |\Psi\rangle \quad , \tag{3.15}$$

with the non-interacting bra state $\langle\Phi|$, and with $|\Psi\rangle$ given by the CCM parametrization of Eq. (3.7), we readily find that the ground-state energy E is given by,

$$E = \tfrac{1}{2}N(N-1)\int\int_{34} v(34)[1+S_2(34)] \ . \tag{3.16}$$

We may similarly derive an equation for $S_2(12)$ by projecting Eq. (3.15) onto the bra state $\langle\Phi|b_0^{\dagger 2}\bar{b}(2)\bar{b}(1)$. After some algebra we find,

$$[t(1)+t(2)]S_2(12)+v(12)+(N-2)\int_3 [v(13)S_2(32)+v(23)S_2(31)]$$

$$+(N-2)(N-3)\int\int_{34} S_2(13)v(34)S_2(42)+v(12)S_2(12)$$

$$+(N-2)S_2(12)\int_3 [v(13)+v(23)]-(2N-3)S_2(12)\int\int_{34} v(34)$$

$$-(2N-3)S_2(12)\int\int_{34} v(34)S_2(34)$$

$$+(N-2)\int_4 [v(14)+v(24)]S_3(124)+\tfrac{1}{2}(N-2)(N-3)\int\int_{34} v(34)S_4(1234)=0 \ , \tag{3.17}$$

where $t(i)\equiv -\nabla_i^2$, and where we continue to use units where $\hbar = 2m = 1$.

In the thermodynamic limit the two terms in the third line of Eq. (3.17) cancel, and we may use the translational invariance to write Eq. (3.17) for $S_2(x)\equiv S_2(\mathbf{x}_1,\mathbf{x}_2)$ with $\mathbf{x}\equiv\mathbf{x}_1-\mathbf{x}_2$,

$$-2\nabla^2 S_2(x)+v(x)+2\rho\int d\mathbf{x}' v(\mathbf{x}-\mathbf{x}')S_2(x')$$

$$+\rho^2\int d\mathbf{x}'\int d\mathbf{x}'' S_2(\mathbf{x}-\mathbf{x}')v(\mathbf{x}'-\mathbf{x}'')S_2(x'')+v(x)S_2(x)$$

$$-2\rho S_2(x)\int d\mathbf{x}' v(x')S_2(x')+2\rho\int d\mathbf{x}' v(\mathbf{x}-\mathbf{x}')S_3(0,\mathbf{x},\mathbf{x}')$$

$$+\tfrac{1}{2}\rho^2\int d\mathbf{x}'\int d\mathbf{x}'' v(\mathbf{x}'-\mathbf{x}'')S_4(0,\mathbf{x},\mathbf{x}',\mathbf{x}'')=0 \ . \tag{3.18}$$

The ground-state energy is given in the same thermodynamic limit as,

$$\frac{E}{N}=\tfrac{1}{2}\rho\int d\mathbf{x}v(x)[1+S_2(x)] \ . \tag{3.19}$$

Equations (3.18) and (3.19) may equivalently be written in the momentum-space representation for $S_2(q)\equiv S_2(\mathbf{q},-\mathbf{q})$ as,

$$2q^2 S_2(q)+v(q)[1+\rho S_2(q)]^2+\int\frac{d\mathbf{q}'}{(2\pi)^d}v(\mathbf{q}-\mathbf{q}')S_2(q')$$

$$-2\rho S_2(q)\int\frac{d\mathbf{q}'}{(2\pi)^d}v(q')S_2(q')+2\rho\int\frac{d\mathbf{q}'}{(2\pi)^d}v(q')S_3(\mathbf{q},\mathbf{q}',-\mathbf{q}-\mathbf{q}')$$

$$+\tfrac{1}{2}\rho^2\int\frac{d\mathbf{q}'}{(2\pi)^d}v(q')S_4(\mathbf{q},-\mathbf{q},\mathbf{q}',-\mathbf{q}')=0 \ , \tag{3.20}$$

and

$$\frac{E}{N} = \tfrac{1}{2}\rho\left[v(q=0) + \int \frac{dq'}{(2\pi)^d} v(q')S_2(q')\right] \quad . \tag{3.21}$$

In Eqs. (3.20) and (3.21) the Fourier transforms $v(q)$ and $S_2(q)$ are defined as,

$$v(q) \equiv \int dx\; e^{iq\cdot x} v(x) \; ; \quad S_2(q) \equiv \int dx\; e^{iq\cdot x} S_2(x) \quad , \tag{3.22}$$

where the latter is consistent with Eqs. (3.13) and (3.14b).

We note that Eqs. (3.18)–(3.21) are exact in the thermodynamic limit, but that they involve coupling of the two-body correlation coefficients to their three- and four-body counterparts. Comparable equations can be derived for the latter, which will also involve couplings to higher-order clusters. In order to use the resulting coupled set of equations in practice, the hierarchy must be broken by a suitable approximation scheme. The most common such scheme is the so-called SUBn scheme in which all correlation operators S_m with $m > n$ are set to zero. It is this scheme upon which we focus in the remainder of this Section, and we return in Sec. 6 to discuss alternatives. Since we are primarily interested in pair correlations we focus attention on the SUB2 scheme, in which we set $S_3 = 0 = S_4$ in Eqs. (3.18) and (3.20). The remaining four terms in Eq. (3.20) now represent respectively: (i) the kinetic energy (KE) contribution; (ii) the term that together with the KE term generates precisely the ring or bubble diagrams summed in the random phase approximation (RPA); (iii) the term that generates the two-boson ladder (LAD) diagrams for the repeated scattering of a pair from out of the condensate; and (iv) the term that generates the self-consistent self-energy insertions on the zero-momentum hole lines, namely the condensate potential (CP) term.

If we now specialize to the one-dimensional Lieb model introduced in Sec. 2, for which $v(q) = 2c$, the SUB2 approximation can be written from Eqs. (3.20) and (3.21) as,

$$[\rho S_2(z)]^2 + \left(z^2 + 4 - 2\frac{e}{\gamma}\right)\rho S_2(z) + \frac{e}{\gamma} = 0 \quad , \tag{3.23}$$

$$e = \gamma + \gamma^{\frac{3}{2}} \int_{-\infty}^{\infty} \frac{dz}{2\pi} \rho S_2(z) \quad , \tag{3.24}$$

in terms of the dimensionless variables e and γ defined in Eqs. (2.11) and (2.12), and a dimensionless momentum variable z defined as $q \equiv \gamma^{\frac{1}{2}}\rho z$. The self-consistent solution for the ground-state energy $e = e(\gamma)$ in this CCM SUB2 approximation is easy to obtain numerically, and results are shown in Table 1. Both the weak- and strong-coupling limits of Eqs. (3.23) and (3.24) can also be found analytically. We readily derive,

$$e_{\rm SUB2} \underset{\gamma\to 0}{\longrightarrow} \gamma - \frac{4}{3\pi}\gamma^{\frac{3}{2}} \quad , \tag{3.25a}$$

$$e_{\rm SUB2} \underset{\gamma\to\infty}{\longrightarrow} \frac{4\gamma}{\gamma^{\frac{1}{2}} + 4} \quad . \tag{3.25b}$$

Whereas Eq. (3.25a) agrees with the exact weak-coupling limit of Eq. (2.14), Eq. (3.25b) is not only in strong disagreement with the constant strong-coupling limit of $\frac{\pi^2}{3}$ for the exact result given by Eq. (2.15), but it is clearly unbounded for large γ. Thus, the CCM SUB2 approximation gives a very poor result in the strong-coupling limit. We shall examine the reasons for this in greater depth below. For the moment

Table 1. Ground-state energy per particle, $E/N = \rho^2 e(\gamma)$, for the one-dimensional Lieb model as a function of the dimensionless coupling constant $\gamma = c/\rho$, with $\rho = N/L$. We show the exact results and the results from the RPA, LAD+SE, and the full CCM SUB2 and SUB3 approximations.

γ	e_{exact}	e_{RPA}	$e_{\text{LAD+SE}}$	e_{SUB2}	e_{SUB3}
0.1	0.0872	0.0866	–	0.0895	–
0.3	0.236	0.230	–	0.251	–
1.0	0.639	0.576	0.632	0.750	0.718
2.0	1.050	0.800	1.136	1.374	–
3.0	1.352	0.795	1.586	1.940	1.80
4.0	1.584	0.605	2.000	2.466	–
5.0	1.769	0.255	2.388	2.963	–
10.0	2.311	-3.421	4.077	5.155	4.50
20.0	2.724	-17.961	–	8.743	–
30.0	2.893	-39.738	–	11.764	9.42
$\to \infty$	$\frac{\pi^2}{3} \approx 3.290$	$-\frac{4}{3\pi}\gamma^{\frac{3}{2}}$	$2(2\gamma)^{\frac{1}{2}}$	$4\gamma^{\frac{1}{2}}$	–

we simply remind the reader that in the limit $\gamma \to \infty$, the Lieb potential becomes a hard-core interaction in the sense that the wave function must vanish when two particles overlap. Indeed, in this one-dimensional case the particles cannot pass through or around each other as $c \to \infty$, so that they behave in this limit like non-interacting fermions. It is precisely because of this (albeit one-dimensional) hard-core property that the Lieb model is of special interest in the present work, since it is well known that the SUBn truncation scheme cannot satisfactorily handle such hard-core systems [4]. The deficiencies of the SUBn schemes in general, and the SUB2 scheme in particular, can thus be well illustrated by the Lieb model, as can the various ways for compensating for them that we discuss below.

Before leaving the SUB2 scheme, however, it is instructive to consider various sub-approximations contained within it. The first of these is the random phase approximation (RPA), which is contained within the CCM SUB2 scheme by ignoring all but the first two terms in Eq. (3.20). In terms of the dimensionless variables introduced previously, the RPA equation is,

$$[\rho S_2(z)]^2 + (z^2+2)\rho S_2(z) + 1 = 0 \ , \tag{3.26}$$

with physical solution,

$$\begin{aligned} \rho S_2(z) &= -\tfrac{1}{2}[z^2 + 2 - (z^4+4z^2)^{\frac{1}{2}}] \\ &= -\frac{(z^4+4z^2)^{\frac{1}{2}} - z^2}{(z^4+4z^2)^{\frac{1}{2}} + z^2} \ . \end{aligned} \tag{3.27a}$$

Insertion of the RPA expression of Eq. (3.27a) into Eq. (3.24) yields the result,

$$e_{\mathrm{RPA}} = \gamma - \frac{4}{3\pi}\gamma^{\frac{3}{2}} \quad , \tag{3.27b}$$

which holds for *all* γ. We note that the RPA expression becomes exact in the $\gamma \rightarrow 0$ limit. This is scarcely surprising since this is just the uniform limit in which the ring diagrams generated by the RPA dominate the ground-state energy.

The next SUB2 sub-approximation that we shall consider is the bare ladder sum (LAD), in which we retain in Eq. (3.17) only the first, second and fifth terms. Equivalently, in Eq. (3.20) we retain only the first and third terms together with the bare potential term $v(q)$ from the second term. However, it is trivial to show that the solution to Eq. (3.20) is now $\rho S_2(z) = -e/\gamma z^2$, which leads to a divergent expression for the energy. This problem is overcome by the inclusion also of the fourth (self-energy or SE) term in Eq. (3.20), in order to renormalise the bare kinetic energy denominators appearing in the ladder approximation. The resulting (LAD+SE) SUB2 sub-approximation is readily expressed in terms of our dimensionless variables as,

$$(z^2 - 2e + 2\gamma)\rho S_2(z) + e = 0 \quad , \tag{3.28a}$$

with a corresponding ground-state energy from Eq. (3.24) given by the cubic equation,

$$8(e-\gamma)^3 + e^2\gamma^2 = 0 \; ; \quad e = e_{\mathrm{LAD+SE}} \quad . \tag{3.28b}$$

In the interesting weak- and strong-coupling limits we obtain,

$$e_{\mathrm{LAD+SE}} \underset{\gamma \rightarrow 0}{\longrightarrow} \gamma \quad , \tag{3.29a}$$

$$e_{\mathrm{LAD+SE}} \underset{\gamma \rightarrow \infty}{\longrightarrow} 2(2\gamma)^{\frac{1}{2}} \quad . \tag{3.29b}$$

From our discussion to date it is clear that the complete neglect in the SUB2 approximation of the coupling terms to three- and four-body clusters in Eqs. (3.18) or (3.20) for the S_2 amplitude is a very poor approximation for the Lieb model at intermediate and large values of γ. One might imagine naively that a possible solution is to proceed to higher SUBn approximations with $n > 2$. For example, in the SUB3 scheme we first derive an equivalent equation to Eq. (3.17) for the S_3 amplitude. This equation contains coupling terms to the S_2, S_4 and S_5 amplitudes. In the SUB3 approximation one now solves simultaneously for S_2 and S_3 by setting S_4 and S_5 to zero. We have also solved the full SUB3 equations (which we do not present here) for the Lieb model, and numerical results are also shown in Table 1. The weak-coupling limit of Eq. (3.25a) is again reproduced in SUB3 approximation. Although we were unable to obtain an analytic form for the energy in the $\gamma \rightarrow \infty$ limit, the numerical evidence strongly suggests that the energy again diverges, although perhaps not quite as rapidly as in the SUB2 case. Although the SUB3 results are marginally better than the SUB2 results, both approximations are extremely poor. We return in Sec. 6 to a more detailed discussion of the reasons why, where we also consider new approximations to improve the CCM performance. Before doing so, however, we discuss two alternative many-body formalisms as an aid to our later discussion.

4. PARQUET THEORY

We now turn our attention to an alternative method of quantum many-body theory, namely the so-called planar or parquet theory [13,17-22]. Since it will be particularly useful for later purposes to draw analogies between the CCM and parquet theory, we derive the basic ingredients of parquet theory below in a way which emphasises their similarities. We stress from the outset, however, that rather than deriving the (two-body) parquet equations in their most general form, we shall make certain simplifying assumptions concerning the locality properties of the fundamental two-body amplitudes that underpin the method. In this way we consider only the so-called local parquet approximation (LPA). Our reasons for making the simplification are threefold. Firstly, the derivation of the full parquet equations is sufficiently complicated that it has often obscured the underlying simplicity of the method. Secondly, the complexity of the full equations usually necessitates further approximations in practice. Finally, although our resulting LPA equations are known [19] from making a suitable localising approximation to the full parquet equations, our greatly simplified direct derivation of the LPA appears not to have appeared previously in the literature.

The LPA is conceptually extremely simple since it contains only two principal ingredients, namely generalized versions of the two-body ladder diagrams familiar from Brueckner-Bethe-Goldstone theory, and generalized versions of the ring diagrams familiar from RPA. As is well known, the ladder diagrams are necessary for a proper description of short-range correlations, at least for potentials with strongly repulsive cores, whereas the ring diagrams are necessary for describing the long-range behaviour. A correct description of the important intermediate-range effects clearly requires some degree of mixing of these two elements. The great strength of parquet theory, even in its present LPA form, is the very high degree to which this is achieved.

From our discussion in Sec. 3 it should be clear to the reader that the CCM also includes at the SUB2 level of approximation all of the bare ring and bare ladder diagrams, as well as many additional diagrams which include a fusion of both elements (e.g., ladders in which the rungs are composed of chains of rings; and rings connected by ladders of two-body interactions). As we shall see later, however, although a large degree of self-consistency is built into the set of rings and ladders iterated together in the CCM SUB2 approximation, nevertheless some important terms of this sort are still missing, which are present in the LPA.

Thus, the basic motivation of the LPA is to include the *full* self-consistent union of ring and ladder diagrams. To this end we introduce two new *local* two-body operators, written in the momentum-space representation as $W(q)$ and $G(q)$. They are extensions of the bare two-body potential $v(q)$, associated with the momentum transfer $\mathbf{q}$, which is henceforth represented diagramatically by a dashed line. The new ingredients $W(q)$ and $G(q)$, denoted by wavy and sawtooth lines respectively, are defined to be *local approximations* to the sum of particle-particle (s-channel) irreducible diagrams and the sum of particle-hole (t-channel) irreducible diagrams, respectively. We use here the standard terminology that a particle or a hole (denoted by a solid line with an arrow pointing upwards or downwards, respectively) are defined with respect to

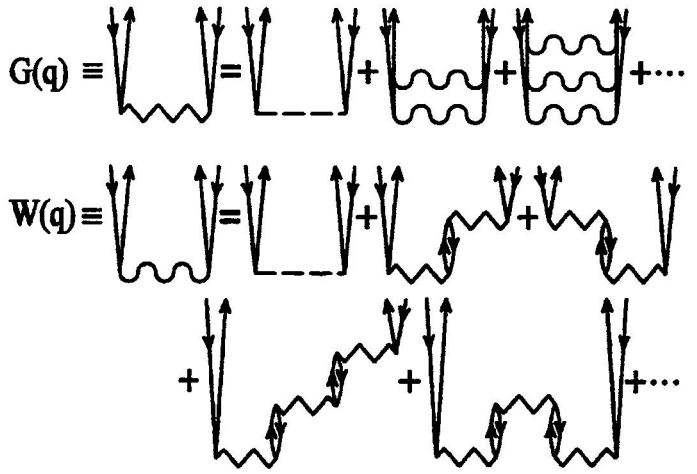

Figure 1. The self-consistent diagrammatic definitions of the LPA amplitudes $G(q)$ and $W(q)$.

the non-interacting zero-momentum condensate state of Eq. (3.8). Furthermore, a diagram is said to be particle-particle (or particle-hole) irreducible if it cannot be made disconnected simply by cutting two internal particle lines (or one internal particle and one internal hole line).

In terms of Goldstone diagrams, the self-consistent definitions of $W(q)$ and $G(q)$ are given in Fig. 1, from which we clearly see that both operators are really nonlocal. We also introduce two related functions $\tilde{G}(q)$ and $\tilde{W}(q)$ which are defined exactly as in Fig. 1 except that the bare potential (driving) term $v(q)$ is replaced respectively by $W(q)$ in the corresponding equation for $\tilde{G}(q)$ and by $G(q)$ in the corresponding equation for $\tilde{W}(q)$. Thus,

$$\tilde{G}(q) = G(q) - v(q) + W(q) \quad , \tag{4.1a}$$

$$\tilde{W}(q) = W(q) - v(q) + G(q) \quad , \tag{4.1b}$$

from which we have trivially the manifest self-consistency relation,

$$\tilde{G}(q) = \tilde{W}(q) \quad , \tag{4.2}$$

which demonstrates the completely symmetric fashion in which the particle-particle and particle-hole channels are treated in the LPA treatment.

Before proceeding we note that the LPA makes no provision for any self-energy insertions which dress the bare propagators, although these can be included in full parquet theory. Furthermore, the above analysis can also be extended to higher orders by replacing the bare potential term $v(q)$ in the two equations represented diagramatically in Fig. 1 by a larger class of fully irreducible diagrams. For present purposes, however, we consider neither of the above extensions.

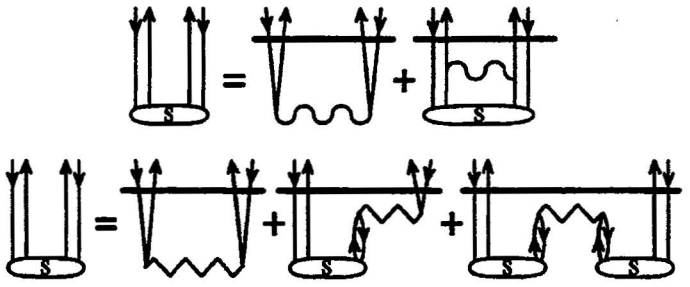

Figure 2. The equations for the basic LPA amplitude $S(q)$.

We now introduce our final LPA amplitude $S(q)$, which is defined as,

$$S(q) \equiv -\frac{1}{2q^2}\tilde{G}(q) = -\frac{1}{2q^2}\tilde{W}(q) \ . \tag{4.3}$$

By recalling that we are using units in which $\hbar^2/2m = 1$, we see that the term $(-2q^2)^{-1}$ in Eq. (4.3) is simply the bare two-particle/two-hole energy denominator. Equation (4.3) has the trivial Fourier transform,

$$\tilde{G}(r) = \tilde{W}(r) = 2\nabla^2 S(r) \ . \tag{4.4}$$

From Fig. 1 and from Eqs. (4.1)-(4.3), we may express the equation determining $S(q)$ in either of the two forms represented in Fig. 2, where the solid horizontal line now represents the energy denominator explicit in Eq. (4.3). They are easily seen to have the algebraic forms,

$$-2q^2 S(q) = W(q) + \int \frac{dq'}{(2\pi)^d} W(\mathbf{q}-\mathbf{q}')S(q') \ , \tag{4.5}$$

$$-2q^2 S(q) = G(q)[1+\rho S(q)]^2 \ . \tag{4.6}$$

We note the strong similarity between Eq. (4.6) and the equation obtained by retaining only the first two terms in Eq. (3.20), where this latter approximation exactly generates the RPA, as described in Sec. 3. Equations (4.1a), (4.3) and (4.6) readily yield the relation,

$$W(q) = v(q) + 2C(q) \ , \tag{4.7}$$

$$C(q) \equiv -q^2 \rho S^2(q) \frac{[2+\rho S(q)]}{[1+\rho S(q)]^2} \ . \tag{4.8}$$

Finally, the insertion of Eq. (4.7) into Eq. (4.5) gives the final equation to determine the basic LPA amplitude $S(q)$,

$$2q^2 S(q) + v(q) + \int \frac{dq'}{(2\pi)^d} v(\mathbf{q}-\mathbf{q}')S(q') + 2C(q)$$

$$+2\int \frac{dq'}{(2\pi)^d} C(\mathbf{q}-\mathbf{q}')S(q') = 0 \ . \tag{4.9}$$

Once $S(q)$ is determined from Eqs. (4.8) and (4.9), the ground-state energy is finally computed from the analogues of Eqs. (3.16) and (3.21),

$$\frac{E}{N} = \tfrac{1}{2}\rho \int dx v(x)[1 + S(x)] = \tfrac{1}{2}\rho \left[v(q=0) + \int \frac{dq}{(2\pi)^d} v(q) S(q) \right] \quad . \tag{4.10}$$

We note that the final LPA equations encapsulated in Eqs. (4.8)-(4.10) are identical to those derived from the full parquet theory [19] by making the localising approximation made here. Before applying the LPA to the Lieb model, we make one further point of considerable importance for later discussion, namely that the LPA presented here is extremely closely related to the optimized Jastrow hypernetted chain (JHNC) approach. Indeed, the diagrammatic content of the two approaches is identical, although the weighting factors of some mixed diagrams do differ [19]. Both methods sum all pure ring and pure ladder diagrams (i.e., those formed with links and rungs respectively equal to the bare two-body potential) with the correct weighting however. Further important work in this area [20] has shown that the optimized JHNC approach is actually *identical* to a similar (but different) local form of exact parquet theory to that considered here.

We now apply the LPA to the Lieb model of Sec. 2. In terms of the previously introduced dimensionless coupling constant γ and energy e, and a dimensionless momentum variable z with $q \equiv \gamma^{\frac{1}{2}} \rho z$, it is not difficult to show that the LPA equations (4.8)–(4.10) can be written in the form,

$$\gamma z^2 \rho S(z) + e + \rho^{-1} C(z) + \gamma^{\frac{1}{2}} \int_{-\infty}^{\infty} \frac{dz'}{2\pi} C(z - z') S(z') = 0 \quad , \tag{4.11a}$$

$$C(z) = -\gamma z^2 \rho^3 S^2(z) \frac{[2 + \rho S(z)]}{[1 + \rho S(z)]^2} \quad , \tag{4.11b}$$

$$e = \gamma + \gamma^{\frac{3}{2}} \int_{-\infty}^{\infty} \frac{dz}{2\pi} \rho S(z) \quad , \tag{4.11c}$$

which may be compared with the corresponding CCM SUB2 equations (3.23) and (3.24). We have solved Eqs. (4.11a-c) numerically and the results are tabulated in Table 2. We observe the excellent agreement with the exact results over the whole range of coupling constants.

In the weak-coupling limit it is not difficult to show that,

$$e_{\mathrm{LPA}} \underset{\gamma \to 0}{\longrightarrow} \gamma - \frac{4}{3\pi} \gamma^{\frac{3}{2}} \quad , \tag{4.12}$$

in agreement with the exact result of Eq. (2.14). Furthermore, to this accuracy, one may shown that the last term in Eq. (4.11a) does not contribute. If we denote the sub-approximation to the LPA where the last term in Eq. (4.9) or (4.11a) is omitted as LPAa, the resulting set of equations (4.11a-c) can be solved exactly. We find,

$$e_{\mathrm{LPAa}} = \gamma \left(1 - \frac{4}{3\pi} e_{\mathrm{LPAa}}^{\frac{1}{2}} \right) \Longleftrightarrow e_{\mathrm{LPAa}} = \gamma + \frac{8\gamma^2}{9\pi^2} - \frac{4\gamma^{\frac{3}{2}}}{3\pi} \left(1 + \frac{4\gamma}{9\pi^2} \right)^{\frac{1}{2}} \quad . \tag{4.13}$$

This LPAa sub-approximation is itself interesting since it turns out to be identical to a sub-approximation to the NIEA of Lieb discussed in Sec. 5 As here, the motivation

Table 2. Ground-state energy per particle, $E/N = \rho^2 e(\gamma)$, for the one-dimensional Lieb model as a function of the dimensionless coupling constant $\gamma = c/\rho$, with $\rho = N/L$. We show the exact results and the results from the local parquet approximation (LPA) and its sub-approximation (LPAa), Lieb's nonlinear integro-differential equation approach (NIEA), and the CCM approximations JSUB2 and HC-JSUB2.

γ	e_{exact}	e_{LPA}	e_{LPAa}	e_{NIEA}	e_{JSUB2}	$e_{\text{HC-JSUB2}}$
0.1	0.08723	0.08725	0.08745	0.08731	–	0.08765
0.3	0.2361	0.2363	0.2379	0.2364	0.2453	0.2387
1.0	0.6392	0.6417	0.6562	0.6382	0.7042	0.6571
3.0	1.352	1.374	1.461	1.329	1.692	1.439
10.0	2.311	2.433	2.843	2.145	3.886	2.649
30.0	2.893	3.150	4.129	2.493	7.289	3.535
100.0	3.162	3.498	5.009	2.593	12.88	4.013
300.0	3.246	3.606	5.355	2.615	20.11	4.173
1000.0	3.277	3.645	5.491	2.622	31.33	4.232
$\to \infty$	$\frac{\pi^2}{3} \approx 3.290$	3.66	$\frac{9\pi^2}{16} \approx 5.552$	2.63	$\approx 3.2\gamma^{\frac{1}{3}}$	4.26

behind the Lieb sub-approximation [23,25] was to keep just those terms needed to obtain the correct second term in the small-γ expansion for the energy. As was pointed out by Lieb [25], Eq. (4.13) actually gives a quite good approximation to e for *all* values of γ. In particular, unlike the CCM SUB2 approximation, it approaches a constant value for large γ,

$$e_{\text{LPAa}} \underset{\gamma\to\infty}{\longrightarrow} \frac{9\pi^2}{16} \quad , \tag{4.14}$$

which may be compared with the exact value from Eq. (2.15). Finally, before turning to Lieb's NIEA method, we remark that the full LPA result for the energy also approaches a constant value as $\gamma \to \infty$. Although we have been unable to calculate this limit analytically, the numerical solution shows that

$$e_{\text{LPA}} \underset{\gamma\to\infty}{\longrightarrow} 3.66 \quad , \tag{4.15}$$

which is only 11% higher than the exact value of $\frac{\pi^2}{3}$.

5. LIEB'S NONLINEAR INTEGRO-DIFFERENTIAL EQUATION APPROACH

Lieb's analysis of the imperfect Bose gas [26,27] begins by defining the exact n-body ground-state subsystem amplitudes characteristic of the configuration-interac-

tion method (CIM). In the same notation as that adopted in Sec. 3, these are defined in terms of the ground-state N-body wave function, $\Psi = \Psi(\mathbf{x}_1, \cdots, \mathbf{x}_N)$, as,

$$\psi_n(1 \cdots n) = \psi_n(\mathbf{x}_1, \cdots, \mathbf{x}_n)$$

$$\equiv \int \cdots \int_{(n+1)\cdots N} \Psi(\mathbf{x}_1, \cdots, \mathbf{x}_N) \Big/ \int \cdots \int_{1\cdots N} \Psi(\mathbf{x}_1, \cdots, \mathbf{x}_N) \ . \qquad (5.1)$$

Integration of both sides of the N-body Schrödinger equation (2.2), with a Hamiltonian comprising a sum of one-body kinetic energies and a potential energy term given by Eq. (3.5), yields the exact relation,

$$E = \tfrac{1}{2} N(N-1) \int \int_{12} v(12)\psi_2(12) \ . \qquad (5.2)$$

To find an equation for $\psi_2(12)$, the Schrödinger equation is integrated over all variables except 1 and 2. This yields,

$$[t(1) + t(2) + v(12)]\psi_2(12) = E\psi_2(12) - 2(N-2) \int_3 \psi_3(123)v(23)$$

$$-\tfrac{1}{2}(N-2)(N-3) \int \int_{34} \psi_4(1234)v(34) \equiv M(12) \ , \qquad (5.3)$$

which is formally equivalent to the CCM Eq. (3.17).

Following Lieb, we now make a careful analysis of the quantity $M(12)$, realizing that although this quantity is expected to be of order unity, its first term in Eq. (5.3) scales like the particle number N. We must therefore be very careful in taking the thermodynamic limit. (Indeed, one of the great attractions of the CCM parametrization of Eq. (3.7) is that this cancellation of $O(N)$ terms is automatically done properly.) By using the cluster property that $\psi_3(123)$ must factorize when particle 1 is far removed from particles 2 and 3, $\psi_3(123) \to P(1)Q(23)$, and the first of the two relations,

$$\int_1 \psi_3(123) = \psi_2(23) \ ; \quad \int \int_{12} \psi_4(1234) = \psi_2(34) \ , \qquad (5.4)$$

which follow immediately from the definition of Eq. (5.1), it follows that to leading order in the volume Ω or particle number N, $P = 1$ and $Q = \psi_2$. Similarly, as particles 1 and 2 become far removed from particles 3 and 4, we find $\psi_4(1234) \to \psi_2(12)\psi_2(34)$. By inserting these leading asymptotic forms into Eq. (5.3), and by making use of Eq. (5.2), we verify that $M(12) \to 0$ as the separation of the two particles tends to infinity.

In order to proceed we now need to obtain the leading corrections to the above asymptotic forms for ψ_3 and ψ_4. Lieb was guided in his further analysis by his unproven assumption that, at least at low enough densities, the functions ψ_3 and ψ_4 would have a superposition form akin to a Jastrow-type product,

$$\psi_3(123) = s[1 + w(12)][1 + w(13)][1 + w(23)] \ , \qquad (5.5)$$

$$\psi_4(1234) = t \prod_{i<j=1}^{4} [1 + z(ij)] \ . \qquad (5.6)$$

The constants s and t and the functions w and z may now be determined from the relations (5.4). By writing ψ_2 as,

$$\psi_2(12) \equiv [1+\Sigma(12)]/(1+\delta)\ ; \quad \delta \equiv \int\int_{12} \Sigma(12)\ , \tag{5.7}$$

we see that $\Sigma(\mathbf{x}_1,\mathbf{x}_2) \equiv \Sigma(\mathbf{x}_1-\mathbf{x}_2) \to 0$ as $|\mathbf{x}_1-\mathbf{x}_2| \to \infty$. Also, $\delta \to 0$ in the bulk limit, $\Omega \to \infty$. We readily find,

$$\begin{aligned} s &= 1-3\delta+o(\Omega^{-1})\ , \\ t &= 1-6\delta+o(\Omega^{-1})\ , \\ w(12) &= \Sigma(12)-\psi_2(12)\int_3 \Sigma(13)\Sigma(23)+o(\Omega^{-1})\ , \\ z(12) &= \Sigma(12)-2\psi_2(12)\int_3 \Sigma(13)\Sigma(23)+o(\Omega^{-1})\ , \end{aligned} \tag{5.8}$$

where the second term in each case is $O(\Omega^{-1})$, and the standard notation $o(x)$ means that the quantity x is of order *lower* than x. The reason for retaining the terms of order Ω^{-1} in Eq. (5.8) is, as explained above, that the first and third terms in $M(12)$ of Eq. (5.3) are both of order N. They cancel to this order, leaving a residue of order unity. The sources of this residue are threefold in the last term of $M(12)$, namely: (i) that $\psi_4(1234)$ goes asymptotically to $\psi(12)\psi(34)+O(\Omega^{-1})$ for particles 3 and 4 far removed from particles 1 and 2; (ii) the contribution to the integral when particle 3 and/or 4 is close to particle 1 and/or 2; and (iii) the presence of the factor $(N-2)(N-3)$ rather than the corresponding $N(N-1)$ in the expression (5.2) for E. By inserting Eqs. (5.5)-(5.7) into Eq. (5.3), and passing to the bulk thermodynamic limit, we obtain the final form of the Lieb NIEA approximation,

$$\begin{aligned} &[t(1)+t(2)]\Sigma(12)+v(12)[1+\Sigma(12)]+2N[1+\Sigma(12)]\int_3 \Sigma(13)[1+\Sigma(23)]v(23) \\ &+N^2[1+\Sigma(12)]\int\int_{34} \Sigma(13)\Sigma(24)\{1+\Sigma(14)+\Sigma(23)+\tfrac{1}{2}\Sigma(14)\Sigma(23)\} \\ &\qquad \times[1+\Sigma(34)]v(34)=0\ . \end{aligned} \tag{5.9}$$

By applying Eq. (5.9) to the Lieb model of Sec. 2 we readily find,

$$\begin{aligned} &-\frac{d^2\Sigma(x)}{dx^2}+\rho e\delta(x)+2\rho^2 e[1+\Sigma(x)]\Sigma(x)+\rho^3 e[1+\Sigma(x)] \\ &\times\left\{\int_{-\infty}^{\infty} dy\Sigma(x-y)\Sigma(y)+2\int_{-\infty}^{\infty} dy\Sigma(x-y)\Sigma^2(y)+\tfrac{1}{2}\int_{-\infty}^{\infty} dy\Sigma^2(x-y)\Sigma^2(y)\right\} \\ &\qquad =0\ , \end{aligned} \tag{5.10a}$$

$$e=\gamma[1+\Sigma(x=0)]\ . \tag{5.10b}$$

We have solved Eq. (5.10) numerically after Fourier transformation into the momentum representation. The results are shown in Table 2. For small values of γ (and

hence e) we expect $\Sigma(x)$ to be small, and it is thus convenient to define new variables $x \equiv e^{-\frac{1}{2}} s/\rho$ and $\Sigma(e^{-\frac{1}{2}} s/\rho) \equiv e^{\frac{1}{2}} \phi(s)$. We readily find,

$$-\frac{d^2\phi}{ds^2} + \delta(s) + [1 + e^{\frac{1}{2}}\phi(s)] \left\{ 2\phi(s) + \int_{-\infty}^{\infty} dt \phi(s-t)\phi(t) \right.$$

$$\left. + 2e^{\frac{1}{2}} \int_{-\infty}^{\infty} dt \phi(s-t)\phi^2(t) + \tfrac{1}{2} e \int_{-\infty}^{\infty} dt \phi^2(s-t)\phi^2(t) \right\} = 0 \ , \qquad (5.11a)$$

$$e = \gamma[1 + e^{\frac{1}{2}}\phi(s=0)] \ . \qquad (5.11b)$$

Thus, we see that to obtain $\phi(s=0)$ to leading order, we may safely neglect the last two terms inside the brace in Eq. (5.11a). In this way we arrive at the equation,

$$-\frac{d^2\phi}{ds^2} + \delta(s) + 2\phi(s) + \int_{-\infty}^{\infty} dt \phi(s-t)\phi(t) = 0 \ , \qquad (5.12)$$

which is readily seen (upon Fourier transformation) to be precisely the same sub-approximation to the NIEA as the sub-approximation LPAa to the LPA discussed in Sec. 4. Thus, the NIEA gives the correct weak-coupling expansion of Eq. (2.14). Further, just like the above (LPAa) sub-approximation to it, the full NIEA also gives a constant value for e as $\gamma \to \infty$. This limiting value is determined numerically to be approximately 2.63, or about 20% lower than the exact value of $\frac{\pi^2}{3}$.

6. COUPLED CLUSTER METHOD: ALTERNATIVE APPROXIMATIONS

It is now of considerable interest to revisit the CCM, and particularly its SUBn approximation scheme, in the light of the LPA and NIEA techniques already discussed. We first recall the exact Eq. (3.17) for the CCM correlation function S_2, where, in the bulk thermodynamic limit, the two terms on the third line cancel each other, and the remaining terms may be represented diagrammatically as in Fig. 3. It is clear by

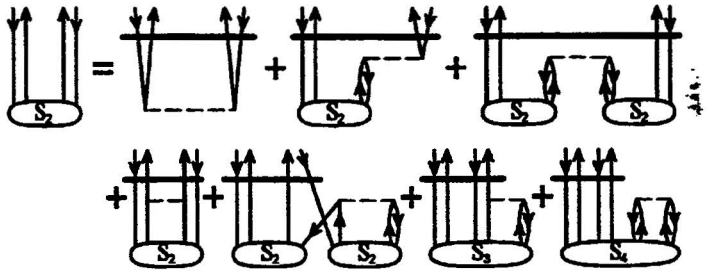

Figure 3. Diagrammatic representation of the exact equation (3.17) for the CCM amplitude S_2 in the bulk thermodynamic limit.

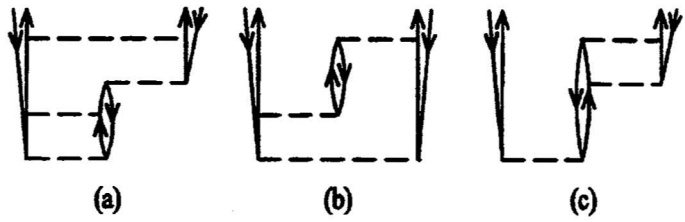

Figure 4. Three Goldstone diagrams which are generated in the LPA scheme. Note that only diagram (a) appears in the CCM SUB2 expansion.

iteration that, as we have already noted, the SUB2 approximation (in which S_3 and S_4 are set to zero) generates all of the pure ring and pure ladder diagrams, as well as many mixed diagrams composed of both ring and ladder elements, such as that illustrated in Fig. 4(a). Nevertheless, there are still many such mixed diagrams which are not present at the SUB2 level of the CCM. Examples are those in Figs. 4(b) and 4(c), which are only contained in the CCM by the inclusion of S_3 (and hence which would only appear in SUBn approximations with $n \geq 3$). By contrast, Figs. 1 and 2 clearly show that all three diagrams in Fig. 4 are generated in the LPA. There are many other such diagrams present in the LPA but absent in CCM SUB2 approximation. Conversely, by neglecting only the self-energy insertions (which merely renormalize the bare propagators), *all* diagrams occurring in SUB2 approximation also occur in the LPA.

The differences between the LPA and CCM SUB2 approximations can also be discussed more formally, by examination of the structure that each method assumes for the ground-state wave function. In the SUB2 approximation we have

$$|\Psi\rangle_{\rm SUB2} = \exp(S_2)|\Phi\rangle \quad , \tag{6.1}$$

where S_2 is a two-body operator with the definite structure that it contains only creation operators with respect to the model state $|\Phi\rangle$. Thus, any two S_2 operators commute. Conversely, in a Jastrow-type approach, such as the LPA, the ansatz for the wave function has the form,

$$|\Psi\rangle_{\rm Jastrow} = \exp(U_2)|\Phi\rangle \quad , \tag{6.2}$$

where U_2 is now a *general* two-body operator, which may have both creation and destruction pieces with respect to $|\Phi\rangle$. Hence, two U_2 operators do not, in general, commute. A consequence is that the Jastrow wave function of Eq. (6.2) is a much more complex object than its CCM SUB2 counterpart of Eq. (6.1).

Expressed in terms of the Goldstone diagram formalism used here, in which time is taken to run in the upwards direction, S_2 is thus a "bottom amplitude" in the sense that the four legs of this four-point function always emerge from the top of its corresponding diagram. This is simply a reflection of the fact that S_2 can only create particles and holes from the vacuum state $|\Phi\rangle$ implicit in the diagrams. By contrast, U_2 can be both a "middle amplitude" and "top amplitude" as well as a "bottom amplitude," as is evident from the representations of the elements W, G

and S in Figs. 1 and 2. Thus, the four legs of the U_2 amplitude may emerge from either the top or the bottom of its diagrammatic equivalent. It is clear that the fact that S_2 is purely a bottom amplitude implies a considerable restriction on the class of diagrams obtained by iteration of its defining equation, by contrast with the Jastrow-type methods. For example, in the LPA scheme, we see that we can build onto every part of the parquet diagrams, and not just the bottom as in the CCM SUB2 scheme.

For all of these reasons it seems likely that the SUBn approximation scheme may, for many purposes, be too drastic. Thus, recalling that Eq. (3.17) (and see Fig. 3) is *exact*, we turn our attention to alternative truncation schemes in which the higher S_n amplitudes are not neglected entirely, but are instead represented in some self-consistent fashion in terms of the lower amplitudes retained. One obvious way of doing this is via the so-called super-SUBn approximation discussed by Robinson [34]. For example, at the super-SUB2 level, we approximate for S_3 and S_4 in the two-body equation (3.17) by reference to the corresponding CCM equations which determine S_3 and S_4. In the three-body equation we retain only those terms which include either S_2 or S_3 alone, or which are simple factorizable products of S_2 and S_3. We thus derive an approximation for S_3 in terms of S_2. A similar treatment of the four-body CCM equation gives S_4 in terms of S_2.

Although we expect that the super-SUBn scheme is likely to be one of the most accurate available, we do not discuss it further here. Instead, for present purposes we choose to develop an alternative, namely the so-called Jastrow SUB2 or JSUB2 scheme, which is motivated by the previous discussion of the LPA and NIEA approaches, and in which we employ a Jastrow-like decomposition of the amplitudes S_3 and S_4.

We thus attempt to equate the CCM and Jastrow forms of the wave function parametrization,

$$\Psi(1\cdots N) \equiv \langle 1\cdots N|\exp\left(\sum_{n=2}^{N} S_n\right)|\Phi\rangle = \prod_{i<j=1}^{N}[1+\sigma(ij)] \quad . \tag{6.3}$$

In fact, we only need to assume the product form for the specific cases $N = 3$ and 4. By choosing $N = 2, 3, 4$ respectively in Eq. (6.3) we find the JSUB2 approximations,

$$\Psi_2(ij)(ij) = 1 + S_2(ij) = 1 + \sigma(ij) \quad , \tag{6.4a}$$

$$\begin{aligned}\Psi_3(ijk) &= 1 + S_2(ij) + S_2(ik) + S_2(jk) + S_3(ijk) \\ &= 1 + \sigma(ij) + \sigma(ik) + \sigma(jk) + \sigma(ij)\sigma(ik) + \sigma(ij)\sigma(jk) \\ &\qquad +\sigma(ik)\sigma(jk) + \sigma(ij)\sigma(ik)\sigma(jk) \quad ,\end{aligned} \tag{6.4b}$$

$$\begin{aligned}\Psi_4(ijkl) &= 1 + S_2(ij) + S_2(ik) + S_2(il) + S_2(jk) + S_2(jl) + S_2(kl) \\ &\qquad +S_2(ij)S_2(kl) + S_2(ik)S_2(jl) + S_2(il)S_2(jk) \\ &\qquad +S_3(ijk) + S_3(ijl) + S_3(ikl) + S_3(jkl) + S_4(ijkl) \\ &= [1+\sigma(ij)][1+\sigma(ik)]\cdots[1+\sigma(kl)] \quad .\end{aligned} \tag{6.4c}$$

Equations (6.4a,b) clearly yield the JSUB2 approximation for S_3,

$$S_3(ijk) = \sigma(ij)\sigma(ik) + \sigma(ij)\sigma(jk) + \sigma(ik)\sigma(jk) + \sigma(ij)\sigma(ik)\sigma(jk) \quad . \tag{6.5}$$

Similarly, Eq. (6.4c) yields the JSUB2 approximation for S_4 in terms of S_2, which we do not write down here due to its length. It includes 16 terms involving products of 3 S_2 functions, 15 involving products of 4 S_2 functions, 6 involving products of 5 S_2 functions, and one term containing a product of all 6 S_2 functions.

By inserting Eq. (6.5) and its counterpart for S_4 into Eq. (3.17) we arrive at the JSUB2 approximation. After a considerable amount of algebra, it may be written in the form,

$$[t(1)+t(2)]\sigma(12) + v(12)[1+\sigma(12)] + 2N[1+\sigma(12)] \int_3 \sigma(13)[1+\sigma(23)]v(23)$$

$$+N^2[1+\sigma(12)] \int\int_{34} \sigma(13)\sigma(24)\{1+\sigma(14)+\sigma(23)+\tfrac{1}{2}\sigma(14)\sigma(23)\}[1+\sigma(34)]v(34)$$

$$+N^2\sigma(12) \int\int_{34} \sigma(13)\sigma(14)[1+\sigma(34)]v(34)$$

$$+2N^2\sigma(12) \int\int_{34} \sigma(13)\sigma(34)v(34)$$

$$+N^2[1+\sigma(12)] \int\int_{34} \sigma(13)\sigma(23)\sigma(34)v(34) = 0 \quad . \tag{6.6}$$

It is interesting to compare Eq. (6.6) with its NIEA counterpart of Eq. (5.9). We see that every term in the NIEA method is also contained in the CCM JSUB2 approach, and the latter also contains some additional terms.

By applying Eq. (6.6) to the Lieb model of Sec. 2 we find,

$$-\frac{d^2\sigma(x)}{dx^2} + \rho e\delta(x) + 2\rho^2 e[1+\sigma(x)]\sigma(x) + \rho^3 e[1+\sigma(x)]$$

$$\times \left\{ \int_{-\infty}^{\infty} dy\sigma(x-y)\sigma(y) + 2\int_{-\infty}^{\infty} dy\sigma(x-y)\sigma^2(y) + \tfrac{1}{2}\int_{-\infty}^{\infty} dy\sigma^2(x-y)\sigma^2(y) \right\}$$

$$+\rho^3 e\sigma(x) \int_{-\infty}^{\infty} dy\sigma^2(y)$$

$$+\rho^3(e-\gamma)\left\{ 2\sigma(x)\int_{-\infty}^{\infty} dy\sigma(y) + [1+\sigma(x)]\int_{-\infty}^{\infty} dy\sigma(x-y)\sigma(y) \right\} = 0 \quad , \tag{6.7a}$$

$$e = \gamma[1+\sigma(x=0)] \quad . \tag{6.7b}$$

We have solved Eq. (6.7a) numerically after Fourier transformation into the momentum representation and the ground-state energy results are shown in Table 2. For small values of γ, the analysis of Eq. (6.7) proceeds exactly as for the NIEA, and we find that the JSUB2 approach gives the correct weak-coupling expansion of Eq. (2.14).

Conversely, in the large-γ limit, the JSUB2 approximation, unlike its NIEA subapproximation, does not converge to a constant value for e, like the exact result of Eq.

(2.15). Instead, from the numerical results, it appears to diverge as $\gamma^{\frac{1}{3}}$. The reason for this difference between the NIEA and JSUB2 results can clearly only lie in the terms in the last three lines of Eq. (6.6) or, equivalently, the last two lines of Eq. (6.7a). Each of these terms emanates from the Jastrow decomposition of the four-body cluster term S_4 in the exact CCM two-body equation (3.17), and we might wonder why there is such a large difference between the two sets of results. The reason is simple. It stems from the hard-core nature of the Lieb model at strong coupling. For hard-core systems it is well known that for a perturbative or diagrammatic treatment to give meaningful results, the whole treatment must be formulated in terms of complete G-matrices. Equivalently, no bare interaction term v must appear in the formulation except in conjunction with an infinite sum of particle-particle ladders.

It is clear from its construction that the LPA possesses the G-matrix property, which partly explains why the method is so successful in treating the Lieb model, especially at large γ. Conversely the CCM SUB2 approximation does not possess this property. This is easily seen from Fig. 4. Thus, whereas diagrams like that in Fig. 4(a) do appear in SUB2 approximation, those like Fig. 4(c) do not. This drawback of the SUB2 scheme, and indeed the whole SUBn hierarchy is well known [2,4]. Indeed, an alternative truncation scheme, the so-called hard-core restricted SUBn (or HC-SUBn), has been used in the nuclear physics context to circumvent this problem. In this scheme only those terms in the SUBn equations are retained which when iterated together lead only to diagrams which are still contained in the original SUBn class when each bare interaction v is replaced by a ladder-summed G-matrix, and when the relative time-orderings of the remaining interactions are kept fixed. Clearly, the HC-SUB2 is just the LAD approximation discussed in Sec. 3, which does not converge for the Lieb model. Furthermore, even higher order HC-SUBn schemes will not take proper account of the ring diagrams.

Let us turn finally to a diagrammatic interpretation of the JSUB2 scheme. The most important thing to note now is that although S_2 as it appears in ordinary SUBn calculations is purely a bottom amplitude, this is not true any longer for its JSUB2 counterpart σ. This is a direct consequence of the Jastrow-like superposition ansatz for S_3 and S_4. For example, the terms $\int_3 \sigma(13)\sigma(23)v(23)$ and $\sigma(12)\int_3 \sigma(13)v(23)$ which appear in the second term in Eq. (6.6) may now be represented diagrammatically as in diagrams (a) and (b) respectively of Fig. 5. Upon iteration, these terms

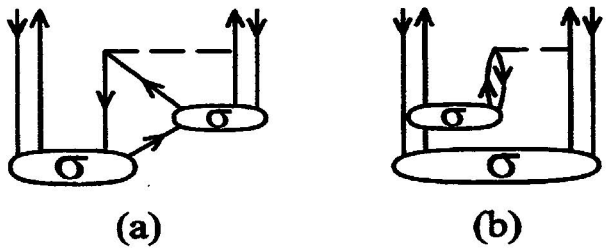

Figure 5. Diagrammatic representation of two terms from the JSUB2 equation (6.6).

clearly generate, for example, the diagrams (c) and (a) respectively of Fig. 4. By similarly iterating together other terms of the JSUB2 equation, we generate many more diagrams which are absent from the SUB2 scheme. However, the complete JSUB2 scheme does not possess the G-matrix property, since for it to do so each bare interaction $v(ij)$ would need to occur in conjunction with the product $v(ij)\sigma(ij)$ and vice versa, i.e., every term involving $v(ij)$ in the defining equation should contain a factor $[1+\sigma(ij)]$. However, it is clear that the terms in the last two lines of Eq. (6.6) do not possess this property. Dropping these terms thereby results in the so-called HC-JSUB2 approximation, to which the NIEA is still a sub-approximation. The HC-JSUB2 results for the Lieb model are also shown in Table 2. They correspond to solving Eq. (6.7a) with the last line omitted. We observe that, as expected, the energy e now approaches a constant value in the $\gamma \rightarrow \infty$ limit. This value is about 30% higher than the exact value.

7. DISCUSSION AND CONCLUSIONS

The incorporation of two-body correlations into the treatment of many-body systems has been attempted many times in the past within different contexts and as part of different more general microscopic theories. Most modern treatments have realized that the dual incorporation of ring and ladder terms is vital for an accurate treatment, but as we have seen their self-consistent union is an extremely subtle matter. Different treatments and different formalisms achieve this union to quite different degrees. In many respects the maximal union has been achieved through parquet theory. This is hardly surprising, since it is the primary motivation for (two-body) parquet theory. Essentially the same degree of mixing is also achieved in the Jastrow variational framework, at least via a localized version of optimal hypernetted chain theory.

Later formal developments of parquet theory have included a possible extension to fermionic systems [35,36]; the inclusion of three-body terms [37]; and parquet perturbation theory for bosons [21] as an expansion in the difference between the exact and approximate propagators, in order to improve systematically upon the local parquet equations. However, despite what is now a rather large corpus of formal developments, the parquet method has not yet been widely applied and tested. This is undoubtedly partly due to the rather complicated derivation and nature of the full parquet equations, before any localising approximations are made. In this respect we hope that our own rather simple and direct derivation of the LPA will prove useful. In particular, it would be extremely useful to repeat the derivation given here for fermions, and we hope to report on this extension elsewhere.

By contrast to parquet theory, the CCM has been very widely applied in physics and chemistry (and see Ref. [6] for a recent review). We have seen how some of the deficiencies of the standard SUBn truncation of the CCM equations, that we have explored in detail here, can be remedied by attempting to mimic within the CCM some of the successes of the LPA and variational treatments employing Jastrow trial wave functions. In particular, we have shown how in the JSUB2 scheme, instead of setting the matrix elements of the higher-order partitions S_3 and S_4 of the correlation operator to zero, as in the standard SUB2 scheme, they have been themselves represented as functions of the S_2 matrix elements. The JSUB2 scheme essentially allocates them

the values they would have if the exact wave function were precisely of Jastrow type. We also note that such an approach can be systematically improved upon by enlarging the Jastrow trial wave functions to the more general Jastrow-Feenberg type. In this way one could derive a general JSUBn scheme, in principle. The success of the JSUB2 scheme also encourages us to explore further the more natural super-SUBn extension of the SUBn scheme which we have already mentioned. In this scheme one does not need to make appeals to other approaches for guidance on how to approximate the higher-order partitions S_m with $m > n$, which are otherwise set to zero in a standard SUBn scheme.

Finally, we note that the comparison made between the methods discussed here has focused on the Lieb model interaction. One reason has been that due to its short-range nature it is a particularly sensitive probe in the strong-coupling limit of methods which do not possess the G-matrix property. Nevertheless, a similar comparison using other potentials would also be useful. An obvious example would be the Coulomb potential, and we shall report comparable results using this potential elsewhere.

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