Variational and diagrammatic evaluations of the ground-state energy of quantum liquids

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The Feynman-Hellmann theorem shows that the exact ground-state energy of a quantum system may be obtained by integrating the potential energy with respect to a coupling constant. For approximation schemes in which the energy is actually calculated from an energy functional, we show that direct and coupling-constant integration evaluations of the energy functional are identical, provided that the energy functional is optimized.

In a previous discussion of summing parquet diagrams to construct the liquid structure function $S(k)$ for Bose systems, we constructed a local approximation to the four-point function $\Gamma(k)$.[1] With this approximation, the self-consistent sum of ladder and ring diagrams (which represents the hallmark of the parquet class) generated a simple Schrödingerlike equation in which the square root of the two-particle distribution function, $\sqrt{g(r)}$, plays the role of the wave function. This equation was seen to be identical to the Euler equation which emerges from Bose hypernetted-chain calculations using the Jackson-Feenberg form of the kinetic energy.[2-4] This established an exact equivalence between the liquid structure function emerging from hypernetted-chain (HNC) variational calculations and that coming from a well-defined approximation to the parquet diagrams; the first such equivalence to be demonstrated. In the present note we demonstrate that the energies calculated by these two techniques are also identical. While the proof is simple, the observation is important in that it completes the demonstration of the equivalence of these approaches to the many-body problem. The proof of equivalence also applies to a larger class of problems.

Using a trial wave function of the Jastrow form, the ground-state energy of a boson system can be written as

$$\frac{E}{A}=\tfrac{1}{2}\rho\int d^3r\,[g(r)V(r)-\tfrac{1}{4}g(r)\nabla^2\ln f^2(r)]\ . \tag{1}$$

Here, f is the usual two-body correlation function and g is the radial distribution function. The exact functional dependence of g on f is extremely complicated; approximation schemes like HNC may produce simpler functional relationships. For the present derivation, we need only assume that the functional relationship between the two does not involve the potential $V(r)$ explicitly.

The Euler equation which minimizes the energy is obtained from a functional variation of E/A with respect to g;

$$\frac{\delta E}{\delta g}=0\ . \tag{2}$$

Again, the specific form of the Euler equation is not relevant to the present arguments.

Let us now look at the variation of the energy with respect to potential strength using Eq. (1). Attaching a subscript α to the f and g to denote their dependence on the strength α, we have

$$\frac{E_\alpha}{A}=\tfrac{1}{2}\rho\int d^3r\,[g_\alpha(r)\alpha V(r)-\tfrac{1}{4}g_\alpha(r)\nabla^2\ln f_\alpha^2(r)]\ , \tag{3}$$

$$\frac{\delta E_\alpha}{\delta g_\alpha}=0\ . \tag{4}$$

Since the α appears as an explicit factor only once, the variation of the energy with α becomes

$$\frac{d}{d\alpha}\left(\frac{E_\alpha}{A}\right)=\tfrac{1}{2}\rho\int d^3r\,g_\alpha(r)V(r)+\frac{1}{A}\int d^3r\,\frac{\delta E_\alpha}{\delta g_\alpha(r)}\frac{dg_\alpha(r)}{d\alpha}. \tag{5}$$

The last term in Eq. (5) vanishes from the stationarity condition of Eq. (4); integration with respect to the coupling constant gives the result

$$\frac{E}{A}=\tfrac{1}{2}\rho\int_0^1 d\alpha\int d^3r\,g_\alpha(r)V(r)\ . \tag{6}$$

This result has the structure of the Feynman-Hellmann theorem and indicates that for the Jastrow problem, coupling-constant integration and direct evaluation of the energy functional are equivalent. For this result to be meaningful, it is necessary that the (approximate) variational wave function and the energy functional adopted actually permit solutions to Eq. (4). The exact relation between g and f from the Jastrow ansatz and the relationship offered by the hypernetted-chain approximation both satisfy this requirement. The generalization of this proof to fermion systems or to situations in which the independent function is defined by a set of parameters is straightforward. The essential features are that the potential should appear once linearly as in Eq. (3) and that the independent function must be optimized.

In the parquet problem,[1] we did not start with an energy functional but relied on coupling-constant integration to evaluate the energy. However, since the parquet and Jastrow HNC results have the same distribution function, it follows directly that the parquet energy can be computed

directly from the Jastrow energy functional.

This result has a number of consequences. It completes the demonstration of the equivalence of hypernetted-chain variational calculations and approximate parquet diagram description of the ground-state properties of boson systems. It makes the useful technical point that, however one chooses to solve the approximate parquet equations in practice, the solution does correspond to an extremum of the parquet energy. Calculations of E/A are thus only quadratically sensitive to errors in g and the four-point function. It also makes it unnecessary to solve the equation for a number of coupling constants.

The above arguments followed extremely general lines. We required merely that the explicit dependence of E/A on the bare interaction, V, was purely linear as it is in Eq. (1). This is of significance when generalizing parquet techniques to systems with spin and spin-dependent interactions.[5] In this case, it is possible to guess the energy functional analogous to Eq. (1) and to verify that it has the structure required by the present proof. The equivalence between the boson parquet and optimized HNC results is unlikely to be repeated in comparing parquet spin-dependent equations with existing variational calculations which do not treat the ring and ladder summations in a self-consistent manner. Indeed, we believe that the diagrammatic arguments which characterize the parquet theory may lead to a less ambiguous but no more complicated approach to the microscopic description of such interesting quantum fluids.

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