Short-Range and Long-Range Forces on a Common Basis in Quantum Crystals

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A theory is developed which allows the determination of the ground-state energy and the phonons of quantum crystals on an equal footing in the collective picture. The central quantity required to dress the lines of the diagrams of the phonons as well as those of the kinetic and potential energy is the phonon self-energy $M(\omega)$. It is approximated in a systematic way, giving the force constants $\Phi$: $M(\omega) = M = \Phi$. This theory is in contrast to those using the T-matrix theory. We show that use of the T-matrix as an effective interaction in phonon calculations leads to an inconsistency.

1. INTRODUCTION

A severe difficulty in a theoretical treatment of quantum crystals is the consistent and equivalent treatment of short-range and long-range correlations. The short-range correlations can be treated, e.g., by T-matrix methods. These have been developed in nuclear physics to overcome the hard core of the two-particle potential. They usually start from a single-particle picture. Long-range correlations, on the other hand, giving rise to phonons, e.g., should better be described in a phonon picture. Here, the unperturbed problem should already contain phonons, being dressed by the anharmonic perturbation.

An equivalent treatment of the short-range and the long-range correlations in quantum crystals requires a combination of these distinct formalisms. On the other hand, the theory has to allow for a simultaneous, self-consistent determination of ground-state and excited state; i.e., the ground-state calculation must be influenced by the phonons and vice versa.

There are several papers concerned with the problem of self-consistently determining ground state and phonons. According to the
method used to overcome the hard core, we can distinguish between two
groups. The first one applies a variational method, i.e., uses Nosanow's
cluster expansion in some way. Here, we are concerned with the second
group, which applies the $T$-matrix method combined with the random phase
approximation (RPA)\textsuperscript{5} or combined with the method of self-consistent
phonons (SCP).\textsuperscript{6,7}

In a previous paper\textsuperscript{10} (hereafter referred to as I) we have pointed out
the difficulties that arise with the use of the $T$-matrix as an effective
interaction in RPA calculations for phonons. These difficulties result from
the fact that in the diagrammatic expansion of $\Delta E_0$ one must not use the true
self-energy to dress the lines, in contrast to the case of phonons. (There are
no skeletons for $\Delta E_0$.) Therefore, the use of the $T$-matrix as an effective
interaction in RPA calculations is not quite consistent. We have shown in I
how to derive a better effective interaction for this purpose.

Following the common practice of adapting the unperturbed Hamiltonian $H_0$
to the true one as well as possible, Glyde and Khanna\textsuperscript{7} succeeded in
building up a $T$-matrix theory where $H_0$ already contains collective excita-
tions. The short-range correlations are treated by approximating the crystal
by a model crystal where only two particles are interacting with the full bare
potential, while all the other particles feel a harmonic interaction. The
harmonic forces, on the other hand, are obtained by the self-consistent
phonon procedure, using the $T$-matrix as an effective interaction. Thus, this
method allows for a simultaneous determination of the ground-state energy
and the collective excitations.

However, the argumentation seems to us somewhat intuitive, especially
concerning the determination of the harmonic potential. Furthermore, it is
to be expected that use of the $T$-matrix as an effective interaction in
determining the self-consistent phonons will lead to the same difficulties as
in the case discussed above. For, it is also the case in a theory where the
unperturbed Hamiltonian already contains harmonic two-particle forces
that the phonon lines in the corresponding diagrams of $\Delta E_0$ (each $T$-matrix
theory concerning quantum crystals is based on the calculation of $\Delta E_0$) must
not be dressed by the entire phonon self-energy $M$. A phonon theory, on the
other hand, should contain the best possible approximation to $M$.

The present paper is concerned with these problems. We give systema-
tic arguments for all approximations and we develop a theory making it
possible to describe ground and excited states on an equal footing.

In Section 2, we repeat the two-particle approximation (TPA) defined
in I. We extend the TPA to the present case where the unperturbed system
already contains collective excitations. Section 3 describes an approxima-
tion to the phonon self-energy. The results are combined to give a self-
consistent theory in Section 4. We compare this theory with that of Glyde