## Editorial Note

Reports on cold fusion have stirred up a lot of activity and emotions in the whole scientific community as well as in political and financial circles. Enthusiasm about its potential usefulness was felt but also severe criticism has been raised. If in such a situation one of the pioneers of modern physics starts to attack the problem in a profound theoretical way we feel that it is our duty to give him the opportunity to explain his ideas and to present his case to a broad and critical audience. We do, however, emphasise that we can take no responsibility for the correctness of either the basic assumptions and the validity of the conclusions nor of the details of the calculations. We leave the final judgment to our readers.

# Nuclear energy in an atomic lattice. 1 

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Evidence is presented for the assertion that an H -ion in a deuterided lattice encounters a relatively narrow Coulomb barrier before fusing to form ${ }^{3} \mathrm{He}$.

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["In this business"] "more is owing to what we call chance - that is... to the observation of events arising from unknown causes - than to any ... preconceived theory."

Joseph Priestley

## Introduction

In a recent note [1] I suggested that the claim of B.S. Pons and M. Fleischmann - to have released nuclear fusion energy by electrolyzing heavy water $\left(\mathrm{D}_{2} \mathrm{O}\right)$ with a palladium cathode - could be true, except that the dominant process would be HD ( $p+d \rightarrow{ }^{3} \mathrm{He}+$ heat), rather than DD (e.g., $d+d \rightarrow{ }^{4} \mathrm{He}+$ heat). The lattice structure of the deuterided palladium plays a vital role in this hypothesis. The presence of the ionic lattice has two effects:

1. Prior to the act of fusion, the lattice coupling diminishes the efficacy of the Coulomb barrier, in a way that strongly favors the HD process over the DD process.
2. After $p d$ fusion begins, the liberated energy is transferred to the multiphonon degrees of freedom of the lattice, rather than to a single high energy photon.

The purpose of this paper is to begin the description of the admittedly crude theoretical considerations that led to my advocacy of the HD hypothesis.

The ultimate judgement of this hypothesis will come, of course, from the outcome of the specific experimental tests that is suggests.

## The lattice

As Albert Einstein knew in 1907 [2], the initial phase of a novel investigation can be hindered by an excess of realism. I have adopted a working picture of the Pd-D metallic lattice that is suggested by the large mass disparity between the alloyed elements:

The Pd-lattice supplies a rigid framework, from which is hung the dynamical D-lattice.

The spatial coordinates and momenta of each of the $N$ D-ions (of mass $M$, and labeled $a$ ), are represented as a linear superposition of phonon modes (labeled $\phi$ ):
$\mathbf{r}_{a}(t)=\mathbf{r}_{a}+\sum_{\phi} \rho_{\phi}\left[\mathbf{y}_{\phi}(t) \mathrm{e}^{\mathrm{i} \mathbf{k}_{\phi} \cdot \mathbf{r}_{a}}+\mathbf{y}_{\phi}^{\dagger}(t) \mathrm{e}^{-\mathrm{i} \mathbf{k}_{\phi} \cdot \mathbf{r}_{a}}\right]$,
$\mathbf{p}_{a}(t)=\sum_{\phi} M \omega_{\phi} \rho_{\phi} \frac{1}{i}\left[\mathbf{y}_{\phi}(t) \mathrm{e}^{\mathrm{i} \mathbf{k}_{\phi} \cdot \mathbf{r}_{a}}-\mathbf{y}_{\sigma}^{\dagger}(t) \mathrm{e}^{-i \mathbf{k}_{\phi} \cdot \mathbf{r}_{\boldsymbol{a}}}\right]$,
with

$$
\begin{align*}
k, l=x, y, z: & {\left[\mathbf{y}_{\phi k}, \mathbf{y}_{\phi^{\prime}}\right]=0 }  \tag{2}\\
& {\left[\mathbf{y}_{\phi k}, \mathbf{y}_{\phi^{\prime} l}^{ \pm}\right]=\delta_{\phi \phi^{\prime}} \delta_{k l} }
\end{align*}
$$

in which the $\mathbf{k}_{\phi}, \omega_{\phi}$ are the phonon propagation vectors and angular frequencies, and
$\rho_{\phi}=\left[\frac{\hbar}{2 M \omega_{\phi} N}\right]^{\frac{1}{2}}$.
The polarization dependence of the phonon spectrum is ignored; there are $N$ three-dimensionally isotropic modes. The orthonormality and completeness expressions for those modes are given by
$\frac{1}{N} \sum_{\phi} \mathrm{e}^{-\mathrm{i} \mathbf{k}_{\phi} \cdot \mathbf{r}_{a}} \mathrm{e}^{\mathrm{i} \mathbf{k}_{\phi} \cdot \mathbf{r}_{a^{\prime}}}=\delta_{a a^{\prime}}$,
$\frac{1}{N} \sum_{a} \mathrm{e}^{-\mathrm{i} \mathbf{k}_{\phi} \cdot \mathbf{r}_{a}} \mathrm{e}^{\mathrm{i} \mathbf{k}_{\phi^{\prime}} \cdot \mathbf{r}_{a}}=\delta_{\phi \phi^{\prime}}$.
The lattice Hamiltonian,
$H_{L}=\sum_{\phi} \hbar \omega_{\phi} \mathbf{y}_{\phi}^{\dagger} \cdot \mathbf{y}_{\phi}$,
supplies equations of motion that are solved by
$\mathbf{y}_{\phi}(t)=\mathrm{e}^{-\mathrm{i} \omega_{\phi} t} \mathbf{y}_{\phi}, \quad \mathbf{y}_{\phi}^{\dagger}(t)=\mathrm{e}^{\mathrm{i} \omega_{\phi} t} \mathbf{y}_{\phi}^{\dagger}$.

## HD reaction

A thermally energetic H -ion, a proton, is in a cell of the Pd- $D$ lattice. This is a proton that will eventually penetrate through to the immediate vicinity of a D-ion, a deuteron, in that cell, thereby forming an excited state of ${ }^{3} \mathrm{He}$. What are the important interactions in this system? Of course the H-ion is coupled electrostatically with the ions outside its own cell and with the Pd-ions in that cell, not to mention the engulfing sea of electrons. These are interactions at the atomic level. But this proton also couples, both electrostatically and through nuclear forces, with the deuteron, in its own cell, with which it will ultimately fuse. In a first overview, surely it is the latter interactions that are central.

Let the Coulomb and nuclear interactions be united in a potential energy $V$, a function of the displacement between $\mathbf{r}$, the position vector of the proton (which is of mass $m$ and carries momentum $\mathbf{p}$ ), and the position vector of that particular deuteron in the $D$-lattice. The lattice interaction-representation, which employs the explicit time dependences of (6), will be adopted, and the equilibrium position of the deuteron is chosen as the spatial origin. Thus, the abbreviated Hamiltonian of this system is
$H=\frac{p^{2}}{2 m}+V\left(\mathbf{r}-\sum_{\phi} \rho_{\phi}\left(\mathrm{e}^{-\mathrm{i} \omega_{\phi} t} \mathbf{y}_{\phi}+\mathrm{e}^{\mathrm{i} \omega_{\phi} t} \mathbf{y}_{\phi}^{\dagger}\right)\right)$.

## Phonon vacuum amplitude

A simple, but not irrelevant situation is that of no initial or final phonons. To solve the Schrödinger equation (in the lattice interaction-representation), one decomposes the wave function,
$\psi=\psi_{0}>_{0}+\psi_{1}, \quad{ }_{0}<\psi_{1}=0$,
where $\psi_{0}$ refers to the persistence of the phonon vacuum symbolized by $>_{0}$. It helps to single out the phonon vacuum term in H , as indicated by
$H=\frac{p^{2}}{2 m}+{ }_{0}<V>_{0}+\left(V-{ }_{0}<V>_{0}\right)$.
Then one has
$i \hbar \frac{\partial}{\partial t} \psi_{0}=\left(\frac{p^{2}}{2 m}+{ }_{0}<V>_{0}\right) \psi_{0}+_{0}<\left(V-_{0}<V>_{0}\right) \psi_{1}$,
and
$i \hbar \frac{\partial}{\partial t} \psi_{1}=\left(\frac{p^{2}}{2 m}+{ }_{0}<V>_{0}\right) \psi_{1}$
$+\left(V-_{0}<V>_{0}\right) \psi_{1}->_{0}<\left(V-{ }_{0}<V>_{0}\right) \psi_{1}$
$+\left(V-_{0}<V>_{0}\right) \psi_{0} \gg_{0}$.
Now, be it a compact notation, or be it the basis of an approximation, one can write the $\psi_{1}$ equation in terms of an effective Hamiltonian, $h$, as
$\left(i \hbar \frac{\partial}{\partial t}-h\right) \psi_{1}=\left(V-_{0}<V>_{0}\right) \psi_{0}>_{0}$,
and arrive at $(\varepsilon \rightarrow+0)$

$$
\begin{align*}
\psi_{1}(t)= & \frac{1}{i \hbar} \int_{-\infty}^{t} \mathrm{~d} t^{\prime} \mathrm{e}^{-\frac{1}{\hbar}\left(t-t^{\prime}\right)(h-i \epsilon)} \\
& \times\left(V-{ }_{0}<V>_{0}\right)\left(t^{\prime}\right) \psi_{0}\left(t^{\prime}\right)>_{0} \tag{13}
\end{align*}
$$

The resulting equation for $\psi_{0}$,
$i \hbar \frac{\partial}{\partial t} \psi_{0}=\left(H^{(1)}+H^{(2)}\right) \psi_{0}$,
has
$H^{(1)}=\frac{p^{2}}{2 m}+{ }_{0}<V>0$
and

$$
\begin{align*}
H^{(2)} \psi_{0}(t)= & \frac{1}{i \hbar} \int_{-\infty}^{t} \mathrm{~d} t^{\prime}{ }_{0}<\left(V-_{0}<V>_{0}\right)(t) \mathrm{e}^{-\frac{i}{\hbar}(t-t)(h-i e)} \\
& \times\left(V-{ }_{0}<V>_{0}\right)\left(t^{\prime}\right)>_{0} \psi_{0}\left(t^{\prime}\right) . \tag{16}
\end{align*}
$$

The next steps are facilitated by writing
$V(\mathbf{r})=\int \frac{(\mathrm{d} \mathbf{q})}{(2 \pi \hbar)^{3}} V(\mathbf{q}) \mathrm{e}^{\frac{i}{\bar{\hbar}} \mathbf{q} \cdot \mathbf{r}}$,
or

$$
\begin{align*}
& V\left(\mathbf{r}-\sum_{\phi} \rho_{\phi}\left(\mathrm{e}^{-\mathrm{i} \omega_{\phi} t} \mathbf{y}_{\phi}+\mathrm{e}^{\mathrm{i} \omega_{\phi} t} \mathbf{y}_{\phi}^{\dagger}\right)\right) \\
& = \\
& =\frac{(\mathrm{d} \mathbf{q})}{(2 \pi \hbar)^{3}} V(\mathbf{q}) \mathrm{e}^{\frac{i}{\hbar} \boldsymbol{q} \cdot \mathbf{r}}  \tag{18}\\
& \quad \times \exp \left[-\frac{i}{\hbar} \mathbf{q} \cdot \sum_{\phi} \rho_{\phi}\left(\mathrm{e}^{-\mathrm{i} \omega_{\phi} t} \mathbf{y}_{\phi}+\mathrm{e}^{\mathrm{i} \omega_{\phi} t} \mathbf{y}_{\phi}^{\dagger}\right)\right],
\end{align*}
$$

which can also be presented as

$$
\begin{align*}
& \int \frac{(\mathrm{d} \mathbf{q})}{(2 \pi \hbar)^{3}} V(\mathbf{q}) \mathrm{e}^{\frac{i}{\hbar} \mathbf{q} \cdot \mathbf{r}} \\
& \times \prod_{\phi} \exp \left[-\frac{i}{\hbar} \rho_{\phi} \mathbf{q} \cdot\left(\mathrm{e}^{-\mathrm{i} \omega_{\phi} t} \mathbf{y}_{\phi}+\mathrm{e}^{\mathrm{i} \omega_{\phi} t} \mathbf{y}_{\phi}^{\dagger}\right)\right] . \tag{19}
\end{align*}
$$

${ }_{0}\langle V\rangle_{0}$
Inasmuch as $N$ should be a very large number, with the implied smallness of $\rho_{\phi}$ of (3), it suffices to retain only the initial terms in the expansion of the individual exponentials that appear in (19):

$$
\begin{align*}
& 1-\frac{1}{\hbar} \rho_{\phi} \mathbf{q} \cdot\left(\mathrm{e}^{-\mathrm{i} \omega_{\phi} t} \mathbf{y}_{\phi}+\mathrm{e}^{\mathrm{i} \omega_{\phi} t} \mathbf{y}_{\phi}^{\dagger}\right) \\
& -\frac{\rho_{\phi}^{2}}{2 \hbar^{2}}\left[\mathrm{e}^{-2 \mathrm{i} \omega_{\phi} t}\left(\mathbf{q} \cdot \mathbf{y}_{\phi}\right)^{2}+\mathrm{e}^{2 i \omega_{\phi} t}\left(\mathbf{q} \cdot \mathbf{y}_{\phi}^{\dagger}\right)^{2}\right. \\
& \left.+2 \mathbf{q} \cdot \mathbf{y}_{\phi}^{\dagger} \mathbf{q} \cdot \mathbf{y}_{\phi}+q^{2}\right] . \tag{20}
\end{align*}
$$

The phonon vacuum state is characterized by
$\mathbf{y}_{\phi}>_{0}=0, \quad{ }_{0}<\mathbf{y}_{\phi}^{\dagger}=0$.
Accordingly, the vacuum expectation value of (20) is

$$
\begin{align*}
1-\frac{\rho_{\phi}^{2}}{2 \hbar^{2}} q^{2} & =\exp \left[-\frac{\rho_{\phi}^{2}}{2 \hbar^{2}} q^{2}\right] \\
& =\exp \left[-\frac{q^{2}}{4 M} \frac{1}{N} \frac{1}{\hbar \omega_{\phi}}\right] . \tag{22}
\end{align*}
$$

Incidentally, although this derivation has been based on the smallness of $1 / N$, the final exponential form is generally valid. The product of all such exponentials introduces
$\frac{1}{N} \sum_{\phi} \frac{1}{\hbar \omega_{\phi}} \equiv\left\langle\frac{1}{\hbar \omega}\right\rangle_{L}$,
the average of $(\hbar \omega)^{-1}$ over the lattice spectrum. Thus, the vacuum expectation value of $V$, as it appears in the Hamiltonian of (7), is
${ }_{0}<V>_{0}=\int \frac{(\mathrm{d} \mathbf{q})}{(2 \pi \hbar)^{3}} V(\mathbf{q}) \mathrm{e}^{\frac{\mathrm{i}}{\mathrm{h}^{\mathbf{q}} \cdot \mathbf{r}}} \exp \left[-\frac{q^{2}}{4 M}\left\langle\frac{1}{\hbar \omega}\right\rangle_{x}\right]$.
An alternative version,
${ }_{0}<V>_{0}=\int(\mathrm{d} \mathbf{R}) \frac{(2 \pi)^{-\frac{3}{2}}}{\Lambda^{3}} \mathrm{e}^{-\frac{3}{2}(R / A)^{2}} V(\mathbf{r}-\mathbf{R})$,
exhibits the characteristic length
$A=\hbar\left[\frac{1}{2 M}\left\langle\frac{1}{\hbar \omega}\right\rangle_{L}\right]^{\frac{1}{2}}$,
in terms of which the Gaussian factor of (24) reads
$\exp \left[-\frac{1}{2}\left(\frac{\Lambda q}{\hbar}\right)^{2}\right]$.
These two representations supply complementary descriptions, which become particularly transparent
for large and small values of $r$ (on the scale set by A), provided there is no undue sensitivity to $r$ in $V$. Thus, for $r \gg A$, the oscillatory structure evident in (24) effectively restrains $q$-values to $q \ll \hbar / \Lambda$, which, according to (24), shows that the lattice is without influence. At the opposite limit, $r \ll \Lambda$, the restriction enforced by (27): $q \leq \hbar / \Lambda$, states that $\exp [(\mathbf{i} / \hbar) \mathbf{q} \cdot \mathbf{r}] \cong 1$; ${ }_{0}<V>_{0}$ becomes independent of $r$. It is not surprising that the implications of these coordinate extremes require only a glance at the coordinate representation (25).

The situation of unscreened Coulomb repulsion,
$V_{c}=\frac{e^{2}}{r}, \quad V_{c}(\mathbf{q})=4 \pi e^{2} \frac{\hbar^{2}}{q^{2}}$,
illustrates these general remarks. Either representation will do, but (25) is more intuitive in asking for the potential of a Gaussian charge distribution:

$$
\begin{align*}
0_{0}<V_{c}>_{0} & =\frac{e^{2}}{r}\left(\frac{2}{\pi}\right)^{\frac{1}{2}} \int_{0}^{r / A} \mathrm{~d} x \mathrm{e}^{-\frac{1}{2} x^{2}} \\
& =\left\{\begin{array}{l}
r \gg A: e^{2} / r \\
r \ll A:(2 / \pi)^{1 / 2}\left(e^{2} / \Lambda\right)
\end{array}\right. \tag{29}
\end{align*}
$$

It is worth noting that, at $r=A$, one is already within $\sim 15 \%$ of the limiting value for $r \ll A$.

The insertion of the deuteron mass for $M$, and of a nominal value of 0.1 eV for the inverse of $\left\langle(h \omega)^{-1}\right\rangle_{L}$, supplies a nominal value for $A$ of (26),
$A \simeq 10^{-9} \mathrm{~cm}$,
and for the limiting value of ${ }_{0}<V_{c}>_{0}$,

$$
\begin{equation*}
\left(\frac{2}{\pi}\right)^{\frac{1}{2}} \frac{e^{2}}{A} \simeq 0.1 \mathrm{keV} \tag{31}
\end{equation*}
$$

It is advisable now to look back at (20) and recognize that, if instead of the phonon vacuum, one selects phonon states of definite, or, indeed, average number $n_{\phi}$, in the sense that
$\left\langle\mathbf{y}_{\phi k}^{\dagger} \mathbf{y}_{\phi l}\right\rangle_{n}=\delta_{k l} n_{\phi}$,
the effect in (24) will be the replacement
$\left\langle\frac{1}{\hbar \omega}\right\rangle_{L} \rightarrow\left\langle\frac{2 n+1}{\hbar \omega}\right\rangle_{L}$.
This will increase the value of $A$, and diminish that of $e^{2} / A$.

## Virtual phonons

Prior to the fusion act, only thermal energy is available to the H-ion and to the D-lattice. Nevertheless, there is a significant effect of the coupling between them that is contained in $H^{(2)}$ of (16).

I revert to the phonon vacuum state and consider, first, $V\left(t^{\prime}\right)>_{0}$, as given in (19), except that the integration variable will be called $\mathbf{q}^{\prime}$, to go with the time variable $t^{\prime}$. The expansion of an individual mode exponential, given in (20), now acts on a vacuum eigenvector only to the right. Accordingly, it acquires an additional term, compared to the initial entry of (22):
$1-\frac{i}{\hbar} \rho_{\phi} \mathbf{q}^{\prime} \cdot \mathrm{e}^{\mathrm{i} \omega_{\phi} t^{\prime}} \mathbf{y}_{\phi}^{\dagger}-\frac{\rho_{\phi}^{2}}{2 \hbar^{2}} q^{\prime 2}$.
On combining the mode factors, and removing the ${ }_{0}<V>_{0}$ contribution, one gets

$$
\begin{align*}
& \left(V-{ }_{0}<V>_{0}\right)\left(t^{\prime}\right)>_{0}=\int \frac{\left(\mathrm{d} \mathbf{q}^{\prime}\right)}{(2 \pi \hbar)^{3}} V\left(\mathbf{q}^{\prime}\right) \mathrm{e}^{\frac{1}{\hbar} \mathbf{q}^{\prime} \cdot \mathbf{r}^{\prime}} \\
& \times\left[\exp \left\{-\frac{\mathrm{i}}{\hbar} \sum_{\phi} \rho_{\phi} \mathbf{q}^{\prime} \cdot \mathrm{e}^{\mathrm{i} \omega_{\phi} t^{\prime}} \mathbf{y}_{\phi}^{ \pm}\right\}-1\right] \\
& \times \exp \left[-\frac{q^{\prime 2}}{4 M}\left\langle\frac{1}{\hbar \omega}\right\rangle_{L}\right]>_{0} \tag{35}
\end{align*}
$$

The adjoint version, referring to time $t$, is

$$
\begin{align*}
& { }_{0}<\left(V-{ }_{0}<V>_{0}\right)(t)=\int \frac{(\mathrm{d} \mathbf{q})}{(2 \pi \hbar)^{3}} V^{*}(\mathbf{q}) \mathrm{e}^{-\frac{1}{\hbar} \mathbf{q} \cdot \mathbf{r}} \\
& \times\left[\exp \left\{\frac{\mathrm{i}}{\hbar} \sum_{\phi} \rho_{\phi} \mathbf{q} \cdot \mathrm{e}^{-\mathrm{i} \omega_{\phi} t^{\prime}} \mathbf{y}_{\phi}\right\}-1\right] \\
& \times \exp \left[-\frac{q^{2}}{4 M}\left\langle\frac{1}{\hbar \omega}\right\rangle_{L}\right] \tag{36}
\end{align*}
$$

On adopting the explicit assumption that the effective Hamiltonian $h$ does not contain phonon variables, one meets a phonon vacuum expectation value that is epitomized by the single mode term

$$
\begin{align*}
& { }_{0}<\left[1+\frac{\mathrm{i}}{\hbar} \rho_{\phi} \mathbf{q} \cdot \mathrm{e}^{-\mathrm{i} \omega_{\phi} t} \mathbf{y}_{\phi}\right]\left[1-\frac{1}{\hbar} \rho_{\phi} \mathbf{q}^{\prime} \cdot \mathrm{e}^{\mathrm{i} \omega_{\phi} t^{\prime}} \mathbf{y}_{\phi}^{\dagger}\right]>_{0} \\
& =1+\frac{\rho_{\phi}^{2}}{\hbar^{2}} \mathbf{q} \cdot \mathbf{q}^{\prime} \mathrm{e}^{-\mathrm{i} \omega_{\phi}\left(t-t^{\prime}\right)} \\
& =1+\frac{\mathbf{q} \cdot \mathbf{q}^{\prime}}{2 M} \frac{1}{N} \frac{1}{\hbar \omega_{\phi}} \mathrm{e}^{-\mathrm{i} \omega_{\phi}\left(t-t^{\prime}\right)} \tag{37}
\end{align*}
$$

These individual mode factors combine into

$$
\begin{align*}
& \exp \left[\frac{\mathbf{q} \cdot \mathbf{q}^{\prime}}{2 M} \frac{1}{N} \sum_{\phi} \frac{1}{\hbar \omega_{\phi}} \mathrm{e}^{-\mathrm{i} \omega_{\phi}\left(t-t^{\prime}\right)}\right] \\
& \equiv \exp \left[\frac{\mathbf{q} \cdot \mathbf{q}^{\prime}}{2 M}\left\langle\frac{1}{\hbar \omega} \mathrm{e}^{-\mathrm{i} \omega\left(t-t^{\prime}\right)}\right\rangle_{L}\right] \tag{38}
\end{align*}
$$

By specializing to an energy eigenstate of energy eigenvalue $E$, so that
$\psi_{0}\left(t^{\prime}\right)=\mathrm{e}^{\frac{1}{\hbar} E\left(t-t^{\prime}\right)} \psi_{0}(t)$,
one can extract an expression for the $H^{(2)}$ of (16), in which one introduces the relative time variable
$\tau=t-t^{\prime}$,
namely,

$$
\begin{align*}
H^{(2)}= & \frac{1}{i \hbar} \int_{0}^{\infty} \mathrm{d} \tau \int \frac{(\mathrm{~d} \mathbf{q})}{(2 \pi \hbar)^{3}} \frac{\left(\mathrm{~d} \mathbf{q}^{\prime}\right)}{(2 \pi \hbar)^{3}} V^{*}(\mathbf{q}) V\left(\mathbf{q}^{\prime}\right) \\
& \times \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} \mathbf{q} \cdot \mathbf{r}} \mathrm{e}^{-\frac{1}{\hbar} \tau(h \cdots E-i \varepsilon)} \mathrm{e}^{\frac{\mathrm{i}}{\hbar} \mathbf{q}^{\prime} \cdot \mathbf{r}} \exp \left[-\frac{q^{2}}{4 M}\left\langle\frac{1}{\hbar \omega}\right\rangle_{L}\right] \\
& \left.\times\left\{\exp \left[\frac{\mathbf{q} \cdot \mathbf{q}^{\prime}}{2 M} / \frac{1}{\hbar \omega} \mathrm{e}^{-\mathrm{i} \omega t}\right\rangle_{L}\right]-1\right\} \\
& \times \exp \left[-\frac{q^{\prime 2}}{4 M}\left\langle\frac{1}{\hbar \omega}\right\rangle_{L}\right] \tag{41}
\end{align*}
$$

A power series expansion of the $\tau$-dependent exponential factor corresponds to considering successive numbers of phonons. The simplest situation occurs for $r \gg A$, where
$q, q^{\prime} \ll \hbar / A$,
or, equivalently [see (26)],
$\frac{q^{2}}{2 M}, \quad \frac{q^{\prime 2}}{2 M} \ll\left(\frac{1}{\hbar \omega}\right\rangle_{L}^{-1}$.
This limits the expansion to the single phonon contribution,
$\exp \left[\frac{\mathbf{q} \cdot \mathbf{q}^{\prime}}{2 M}\left\langle\frac{1}{\hbar \omega} \mathrm{e}^{-\mathrm{i} \omega \tau}\right\rangle_{L}\right]-1 \cong \frac{\mathbf{q} \cdot \mathbf{q}^{\prime}}{2 M}\left(\frac{1}{\hbar \omega} \mathrm{e}^{-\mathrm{i} \omega t}\right\rangle_{L}$.
Along the same lines as (43), but possibly somewhat more stringent, is the assumption that the $h$ spectrum for the state $\exp \left[(\mathbf{i} / \hbar) q^{\prime} \cdot \mathbf{r}\right] \psi_{0}(\mathbf{r})$ differs so little from $E$ that only the phonon energy $\hbar \omega$ need be considered. This yields

$$
\begin{align*}
H^{(2)} \simeq- & {\left[\int \frac{(\mathrm{d} \mathbf{q})}{(2 \pi \hbar)^{3}} V^{*}(\mathbf{q}) \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} \mathbf{q} \cdot \mathbf{r}} \mathbf{q}\right] } \\
& \cdot\left[\int \frac{\left(\mathrm{d} \mathbf{q}^{\prime}\right)}{(2 \pi \hbar)^{3}} V\left(\mathbf{q}^{\prime}\right) \mathrm{e}^{\frac{1}{\hbar} \mathbf{q}^{\prime} \cdot \mathbf{r}} \mathbf{q}^{\prime}\right] \\
& \cdot \frac{1}{2 M}\left\langle\left(\frac{1}{\hbar \omega}\right)^{2}\right\rangle_{L}=-(\boldsymbol{V} V)^{2} \frac{1}{2 M}\left\langle\frac{1}{\omega^{2}}\right\rangle_{L} \tag{45}
\end{align*}
$$

One can, of course, arrive at this limiting form in a more elementary way, where it appears as
$-\nabla V \cdot \sum_{\phi} \rho_{\phi} \frac{1}{\hbar \omega_{\phi}} \rho_{\phi} \nabla V$.
In the example of the unscreened Coulomb potential, (45) reads
$H^{(2)} \simeq-\frac{e^{2}}{r}\left(\frac{\Lambda}{r}\right)^{3} \frac{2 \Lambda}{\hbar^{2} / M e^{2}}\left\langle\frac{1}{\omega^{2}}\right\rangle_{L}\left(\frac{1}{\langle 1 / \omega\rangle_{L}}\right)^{2}$,
or, equivalently,
$H^{(2)} \simeq-\frac{M e^{4}}{2 \hbar^{2}} 4\left(\frac{\Lambda}{r}\right)^{4}\left\langle\frac{1}{\omega^{2}}\right\rangle_{L}\left(\frac{1}{\langle 1 / \omega\rangle_{L}}\right)^{2}$,
where one recognizes the Bohr energy associated with mass $M$.

If, à la Einstein, the lattice spectrum were assumed to be sharply peaked at a single frequency, the product of the two lattice averages would be unity. At the opposite limit - a spectral density proportional to $\omega^{2}$ - this product is no more than $4 / 3$.

The Bohr radius associated with mass $M$ that appears in (47) is $\sim 10^{-12} \mathrm{~cm}$ for the deuteron mass. Accordingly [see (30)]
$\frac{2 \Lambda}{\hbar^{2} / M e^{2}} \sim 10^{3}$,
and one can present the outcome as
$r \gg A:-\frac{H^{(2)}}{e^{2} / r} \sim\left(\frac{10 A}{r}\right)^{3}$.

Here, at least, is a suggestion that, already at distances as large as $10 \Lambda \sim 10^{-8} \mathrm{~cm}$, the energy of attraction, $H^{(2)}$, begins to reduce significantly the Coulomb energy of repulsion.

## References

[^0]
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