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Phonon representations

(lattice/spectrum)

JULIAN SCHWINGER

Department of Physics, University of California, Los Angeles, CA 90024

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ABSTRACT The gap between the nonlocalized lattice-phonon description and the localized Einstein oscillator treatment is filled by transforming the phonon Hamiltonian back to the particle variables. The particle-coordinate, normalized, wave function for the phonon vacuum state is exhibited.

The lattice phonon is a spatially nonlocalized concept. There are circumstances, however, that require its combination with other, localized, phenomena. Then, one might wish to return to a description that uses the more localized interactions among the lattice constituents. Such interactions may not be very well known, however, and, in contrast with the phonon spectrum, are not subject to direct measurement. It would be of some utility, therefore, to transform back from the phonon description in order to realize the localized treatment of the lattice particles.

In the interests of minimizing notational problems, the distinction between longitudinal and transverse polarizations will be set aside, so that each phonon mode, labeled ϕ, and characterized by angular frequency ω_ϕ and propagation vector $\mathbf{k}_\phi$, will be three-dimensionally degenerate. This is conveyed by the following Hamiltonian, referring to the linear displacement regime, which is expressed in terms of the phonon annihilation operator $\mathbf{y}_\phi$ and the adjoint creation operator $\mathbf{y}_\phi^\dagger$, as

$$\mathscr{H} = \sum_\phi \hbar\omega_\phi \mathbf{y}_\phi^\dagger \cdot \mathbf{y}_\phi. \quad [1]$$

Given N equilibrium positions, $\mathbf{r}_{0a}$, one introduces the dynamical position vectors

$$\mathbf{r}_a = \mathbf{r}_{0a} + \sum_\phi \rho_\phi (e^{i\mathbf{k}_\phi\cdot\mathbf{r}_{0a}}\mathbf{y}_\phi + e^{-i\mathbf{k}_\phi\cdot\mathbf{r}_{0a}}\mathbf{y}_\phi^\dagger), \quad [2]$$

along with the momenta for particles of mass M,

$$\mathbf{p}_a = \sum_\phi M\omega_\phi\rho_\phi \frac{1}{i}(e^{i\mathbf{k}_\phi\cdot\mathbf{r}_{0a}}\mathbf{y}_\phi - e^{-i\mathbf{k}_\phi\cdot\mathbf{r}_{0a}}\mathbf{y}_\phi^\dagger), \quad [3]$$

where

$$\rho_\phi = \left(\frac{\hbar}{2M\omega_\phi N}\right)^{1/2} \quad [4]$$

From the commutation relations of the non-Hermitian phonon operators, as illustrated by $(k, l = x, y, z)$,

$$[y_{\phi k}, y_{\phi' l}^\dagger] = \delta_{kl}\delta_{\phi\phi'}, \quad [5]$$

one gets the required coordinate-momentum commutation relations,

$$\frac{1}{i\hbar}[\mathbf{r}_{ak}, \mathbf{p}_{bl}] = \delta_{kl}\delta_{ab}, \quad [6]$$

as a consequence of the phonon property

$$\frac{1}{N}\sum_\phi e^{i\mathbf{k}_\phi\cdot(\mathbf{r}_{0a}-\mathbf{r}_{0b})} \equiv \langle e^{i\mathbf{k}\cdot(\mathbf{r}_{0a}-\mathbf{r}_{0b})}\rangle = \delta_{ab}. \quad [7]$$

The notation introduced here for a spectral average, ⟨⟩, will occur again.

The inverses of the relations **2** and **3** are given by

$$\mathbf{y}_\phi = \sigma_\phi \sum_a \left[(\mathbf{r}-\mathbf{r}_0)_a + \frac{i}{M\omega_\phi}\mathbf{p}_a\right]e^{-i\mathbf{k}_\phi\cdot\mathbf{r}_{0a}}, \quad [8]$$

along with its adjoint,

$$\mathbf{y}_\phi^\dagger = \sigma_\phi \sum_a \left[(\mathbf{r}-\mathbf{r}_0)_a - \frac{i}{M\omega_\phi}\mathbf{p}_a\right]e^{i\mathbf{k}_\phi\cdot\mathbf{r}_{0a}}, \quad [9]$$

where

$$\sigma_\phi = (2N\rho_\phi)^{-1} = \left(\frac{M\omega_\phi}{2\hbar N}\right)^{1/2} \quad [10]$$

The new form of the Hamiltonian **1** that Eqs. **8** and **9** supply is

$$\mathscr{H} = \sum_a \left(\frac{\mathbf{p}_a^2}{2M} - \frac{3}{2}\hbar\langle\omega\rangle\right) + \sum_{ab}\frac{M}{2}(\mathbf{r}-\mathbf{r}_0)_a\cdot\Omega_{ab}^2(\mathbf{r}-\mathbf{r}_0)_b, \quad [11]$$

where

$$\Omega_{ab}^2 = \langle\omega^2 e^{i\mathbf{k}\cdot(\mathbf{r}_{0a}-\mathbf{r}_{0b})}\rangle. \quad [12]$$

The notation Ω^2 has a matrix significance, based on

$$\Omega_{ab} = \langle\omega e^{i\mathbf{k}\cdot(\mathbf{r}_{0a}-\mathbf{r}_{0b})}\rangle. \quad [13]$$

Indeed, with the assistance of the lattice property that is complementary to Eq. **7**,

$$\frac{1}{N}\sum_a e^{i(\mathbf{k}_\phi-\mathbf{k}_{\phi'})\cdot\mathbf{r}_{0a}} = \delta_{\phi\phi'}, \quad [14]$$

one gets

$$\begin{aligned}\Omega_{ac}^2 &= \sum_b \Omega_{ab}\Omega_{bc}\\ &= \frac{1}{N}\sum_{\phi\phi'}\omega_\phi\omega_{\phi'}\frac{1}{N}\sum_b e^{i\mathbf{k}_\phi\cdot(\mathbf{r}_{0a}-\mathbf{r}_{0b})}e^{i\mathbf{k}_{\phi'}\cdot(\mathbf{r}_{0b}-\mathbf{r}_{0c})}\\ &= \frac{1}{N}\sum_\phi \omega_\phi^2 e^{i\mathbf{k}_\phi\cdot(\mathbf{r}_{0a}-\mathbf{r}_{0c})},\end{aligned} \quad [15]$$

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which is the content of Eq. **12**. The immediate generalization to any positive integer n is

$$\Omega^n_{ab} = \langle \omega^n e^{i\mathbf{k}\cdot(\mathbf{r}_{0a}-\mathbf{r}_{0b})}\rangle. \quad [16]$$

The specializations

$$\Omega^2_{aa} = \langle \omega^2 \rangle$$

and

$$\Omega^2_{ab}(a \neq b) = \langle(\omega^2 - \langle\omega^2\rangle)e^{i\mathbf{k}\cdot(\mathbf{r}_{0a}-\mathbf{r}_{0b})}\rangle, \quad [17]$$

convert Eq. **11** into

$$\mathcal{H} = \sum_a \left[\frac{\mathbf{p}_a^2}{2M} + \frac{M}{2}\langle\omega^2\rangle(\mathbf{r}-\mathbf{r}_0)_a^2 - \frac{3}{2}\hbar\langle\omega\rangle\right] + \sum_{a\neq b}\frac{M}{2}(\mathbf{r}-\mathbf{r}_0)_a \cdot \Omega^2_{ab}(\mathbf{r}-\mathbf{r}_0)_b. \quad [18]$$

This directs attention to the limit in which the spectrum is monochromatic: $\omega^2 = \langle\omega^2\rangle = \langle\omega\rangle^2$, where the Einstein description in terms of independent oscillators emerges. The phonon vacuum state for this circumstance is known from the oscillator ground-state wave function:

$$\langle\{\mathbf{r}\}|0\rangle = \prod_a \left(\frac{M\omega}{\pi\hbar}\right)^{3/4} \exp\left[-\frac{M\omega}{2\hbar}(\mathbf{r}-\mathbf{r}_0)_a^2\right]. \quad [19]$$

What replaces this for a general phonon spectrum?

According to Eq. **8**, the vacuum condition, $\mathbf{y}_\phi|0\rangle = 0$, implies that

$$\sum_b \left[\frac{M\omega_\phi}{\hbar}(\mathbf{r}-\mathbf{r}_0)_b + \frac{i}{\hbar}\mathbf{p}_b\right] e^{-i\mathbf{k}_\phi\cdot\mathbf{r}_{0b}}|0\rangle = 0. \quad [20]$$

With the aid of the phonon property (Eq. **7**), this is converted into

$$\left[\frac{i}{\hbar}\mathbf{p}_a + \frac{M}{\hbar}\sum_b \Omega_{ab}(\mathbf{r}-\mathbf{r}_0)_b\right]|0\rangle = 0 \quad [21]$$

or

$$\left[\nabla_a + \frac{M}{\hbar}\sum_b \Omega_{ab}(\mathbf{r}-\mathbf{r}_0)_b\right]\langle\{\mathbf{r}\}|0\rangle = 0, \quad [22]$$

in the notation of Eq. **13**. The solution of the latter set of equations is

$$\langle\{\mathbf{r}\}|0\rangle = C\exp\left[-\frac{M}{2\hbar}\sum_{ab}(\mathbf{r}-\mathbf{r}_0)_a \cdot \Omega_{ab}(\mathbf{r}-\mathbf{r}_0)_b\right], \quad [23]$$

which, in the monochromatic situation—where Ω_{ab} equals $\omega\delta_{ab}$—reproduces the structure of Eq. **19**.

Now the normalization condition reads

$$1 = C^2\left(\frac{\pi\hbar}{M}\right)^{3N/2}(\det\Omega)^{-3/2}. \quad [24]$$

The differential definition of the determinant in terms of the trace is

$$\delta\log(\det\Omega) = \mathrm{tr}(\Omega^{-1}\delta\Omega). \quad [25]$$

With the permissible extension of Eq. **16** to $n = -1$, one gets

$$(\Omega^{-1}\delta\Omega)_{ab} = \left\langle\frac{\delta\omega}{\omega}e^{i\mathbf{k}\cdot(\mathbf{r}_{0a}-\mathbf{r}_{0b})}\right\rangle \quad [26]$$

and then

$$\mathrm{tr}(\Omega^{-1}\delta\Omega) = N\left\langle\frac{\delta\omega}{\omega}\right\rangle = \delta(N\langle\log\omega\rangle). \quad [27]$$

The outcome,

$$\det\Omega = \langle\omega\rangle^N \exp\left(N\left\langle\log\frac{\omega}{\langle\omega\rangle}\right\rangle\right), \quad [28]$$

is independent of $\langle\omega\rangle$, which appears as a matter of convenience.

Thus, one finds that

$$C = c^N, \quad c = \left(\frac{M\langle\omega\rangle}{\pi\hbar}\right)^{3/4}\exp\left(-\frac{3}{4}\left\langle\log\frac{\langle\omega\rangle}{\omega}\right\rangle\right), \quad [29]$$

where the logarithm is so written in the anticipation that its spectral average is positive. Consider, for example, the situation of a narrow spectral range that is symmetrical about $\langle\omega\rangle$. Then, if one writes $\omega = \langle\omega\rangle(1+x)$, the symmetry implies that

$$\left\langle\log\frac{\langle\omega\rangle}{\omega}\right\rangle = \left\langle\log\frac{1}{1+x}\right\rangle = \left\langle\log\frac{1}{1-x}\right\rangle = \frac{1}{2}\left\langle\log\frac{1}{1-x^2}\right\rangle > 0. \quad [30]$$

On the other hand, consider the asymmetrical Debye spectrum, with a spectral density proportional to ω^2, up to a cutoff frequency. With the latter chosen as the ω unit, one has

$$\left\langle\log\frac{\langle\omega\rangle}{\omega}\right\rangle = \int_0^1 d\omega\,\omega^2\,3\log\frac{3}{4\omega} = \frac{1}{3} - \log\frac{4}{3} = 0.046 > 0. \quad [31]$$