Annotations of Peschel

Shi Feng
(Dated: May 22, 2021)

TBW

I.

Consider a purely bosonic model, a chain of L harmonic oscillator with frequency ω_0, coupled together by springs. It has a gap in the phonon spectrum and is a non-critical integrable system. The Hamiltonian reads

$$H = \sum_{i=1}^{L}\left(-\frac{1}{2}\frac{\partial^2}{\partial x_i^2} + \frac{1}{2}\omega_0^2 x_i^2\right) + \sum_{i=1}^{L-1}\frac{1}{2}\kappa(x_{i+1}-x_i)^2 \tag{1}$$

Peschel parameterized it by $\omega_0 = 1-\kappa$, so that if $\kappa = 0$ the Hamiltonian is digonal under boson occupation number, and there is no dispersion (only one mode ω_0) and the system is gapped. If $\kappa \to 1$ (thus $\omega_0 \to 0$), there will only be acoustic phonon excitations and the system become gapless.

A. 2 particle problem

As the simplest example let us scrutinize the 2-particle problem. Its Hamiltonian reads

$$H = \frac{1}{2}\frac{\partial^2}{\partial x_1^2} + \frac{1}{2}\frac{\partial^2}{\partial x_2^2} + \frac{1}{2}\omega_0^2 x_1^2 + \frac{1}{2}\omega_0^2 x_2^2 + \frac{\kappa}{2}(x_1-x_2)^2 \tag{2}$$

We don't want off-diagonal terms like $x_1 - x_2$, so we do the following transformation:

$$v = (x_1+x_2)/\sqrt{2},\;\; u = (x_1-x_2)/\sqrt{2} \quad\Longleftrightarrow\quad x_1 = (v+u)/\sqrt{2},\;\; x_2 = (v-u)/\sqrt{2} \tag{3}$$

I like the factor of $\sqrt{2}$ because of its reciprocal symmetry (also the transformation belongs to $O(2)$ so that $\sum_i x_i^2$ remain the same form). Then the potential energy becomes

$$\frac{1}{2}\omega_0 x_1^2 + \frac{1}{2}\omega_0 x_2^2 + \frac{\kappa}{2}(x_1-x_2)^2 = \frac{1}{2}\omega_0 v^2 + \frac{1}{2}\omega_0 u^2 + \frac{\kappa}{4}u^2 \tag{4}$$

$$H = \frac{1}{2}\frac{\partial^2}{\partial u^2} + \frac{1}{2}\left(\omega_0^2 + \frac{\kappa}{2}\right)u^2 + \frac{1}{2}\frac{\partial^2}{\partial v^2} + \frac{1}{2}\omega_0^2 v^2 \equiv H_u + H_v \tag{5}$$

which describes two de-coupled harmonic oscillators. Since $[H, H_u] = [H, H_v] = [H_u, H_v] = 0$, wavefunctions of two harmonic modes can be measured simultanously, and their corresponding wavefunctions become separable. The ground state of a 1D harmonic oscillator with angular frequency ω is

$$\Psi(x) = \left(\frac{\omega}{\pi}\right)^{1/4}\exp\!\left(-\frac{\omega}{2}x^2\right)\exp\!\left(-i\frac{\omega}{2}t\right) \tag{6}$$

therefore, if define $\Omega^2 \equiv (1/2)(\omega_0^2 + \kappa/2)$, the joint wavefunction of normal modes is

$$\Psi(u,v) = C\exp\!\left(-\frac{\Omega}{2}u^2 - \frac{\omega_0}{2}v^2\right) \tag{7}$$

where C is a normalization constant. Next we are going to calculate the reduced density matrix of the state by tracing out one of the oscillators in the original coordiate. For example, let us trace out x_1 for the density matrix of x_2:

$$\begin{aligned}
\rho_2(x_2,x_2') &= \int_{-\infty}^{\infty} dx_1 \Psi^*(x_1,x_2')\Psi(x_1,x_2) \\
&\propto \int_{-\infty}^{\infty} dx_1 \exp\Big(-\frac{\Omega}{4}(x_1-x_2')^2 - \frac{\omega_0}{4}(x_1+x_2')^2\Big)\exp\Big(-\frac{\Omega}{4}(x_1-x_2)^2 - \frac{\omega_0}{4}(x_1+x_2)^2\Big) \\
&= \exp\Big\{-\Big(\frac{\omega_0+\Omega}{4}\Big)(x_2^2+x_2'^2)\Big\}\int_{-\infty}^{\infty} dx_1 \exp\Big\{-\Big(\frac{\omega_0+\Omega}{2}\Big)x_1^2 + \Big[\Big(\frac{\Omega-\omega_0}{2}\Big)(x_2+x_2')\Big]x_1\Big\} \\
&\propto \exp\Big\{-\Big(\frac{\omega_0+\Omega}{4}\Big)(x_2^2+x_2'^2)\Big\}\exp\Big\{\frac{(\Omega-\omega_0)^2}{8(\omega_0+\Omega)}(x_2+x_2')^2\Big\} \\
&= \exp[-\gamma(x_2+x_2')/2 + \beta x_2 x_2']
\end{aligned} \tag{8}$$

where

$$\beta = \frac{(\Omega-\omega_0)^2}{4(\omega_0+\Omega)}, \quad \gamma = \frac{\omega_0^2+\Omega^2+6\omega_0\Omega}{4(\omega_0+\Omega)}, \quad \gamma-\beta = \frac{2\omega_0\Omega}{\omega_0+\Omega}.$$

and the normalized reduced density matrix is

$$\rho_2(x_2,x_2') = \sqrt{\frac{\gamma-\beta}{\pi}}\exp\Big[-\frac{\gamma}{2}(x_2^2+x_2'^2) + \beta x_2 x_2'\Big] \tag{9}$$

To calculate von-Neumann entanglement entropy we need to solve the following eigenvalue problem:

$$\int_{-\infty}^{\infty} dx' \rho_2(x,x') f_n(x') = p_n f_n(x) \tag{10}$$

whereby the EE can obtained by $S = -\sum_n p_n \log p_n$. The solution can be guessed:

$$p_n = (1-\xi)\xi^n \tag{11}$$

$$f_n(x) = H_n(\alpha^{1/2}x)\exp\big(-\alpha x^2/2\big) \tag{12}$$

where H_n is the Hermit polynomial, $\alpha = (\gamma^2-\beta^2)^{1/2}$, $\xi = \beta/(\gamma+\alpha)$. Then EE can be calculated by

$$S = -\sum_n (1-\xi)\xi^n \log(1-\xi)\xi^n \tag{13}$$

B. N particles

Using PBC, the Hamiltonian can be written as

$$H = \sum_{i=1}^{N}\Big(-\frac{1}{2}\frac{\partial^2}{\partial x_i^2} + \frac{1}{2}\omega_0^2 x_i^2 + \frac{\kappa}{2}(x_i - x_{i+1})^2\Big), \qquad x_{N+1} = 0, \tag{14}$$

$$\equiv \frac{1}{2}p^T M p + \frac{1}{2}x^T K x, \tag{15}$$

where $M = I$ is diagonal and K is a real symmetric $N \times N$ matrix with positive eigenvalues,

$$K = \begin{pmatrix} \kappa' & -\kappa & 0 & \cdots & 0 \\ -\kappa & \kappa' & -\kappa & \ddots & \vdots \\ 0 & -\kappa & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \kappa' & -\kappa \\ 0 & \cdots & 0 & -\kappa & \kappa' \end{pmatrix} \tag{16}$$

with $\kappa_i' = \omega_0^2 + \kappa$. By choosing a basis which diagonalizes the matrix K, the hamiltonian can be express as the sum of uncoupled harmonic oscillators hamiltonian. That is

$$X^T U^T \left(UKU^T\right) UX \equiv Y^T K_D Y, \qquad \text{with } U^T U = I \tag{17}$$

where K_D is a diagonal matrix whose elements are the square of angular frequencies ω_i^2 of i-th normal modes. The resultant joint wavefunction takes the form

$$\Psi(\mathbf{x}) \propto \exp\left\{-\frac{Y^T\sqrt{K_D}T}{2}\right\} = \exp\left\{-\frac{X^T(U^T\sqrt{K_D}U)X}{2}\right\} \equiv \exp\left\{-\frac{X^T A X}{2}\right\} \tag{18}$$

where we defined the coupling matrix $A \equiv U^T\sqrt{K_D}U$ whose elements are the energies (characteriztic frequencies e.g. $\omega_{ij}x_i x_j$) of bonds between oscillators. The normalized wavefunction then reads

$$\Psi(\mathbf{x}) = \left(\frac{\det(A)}{\pi^N}\right)^{\frac{1}{4}} \exp\left\{-\frac{X^T A X}{2}\right\} \tag{19}$$

Now that we have the phsyical intuition, let us trim and clarify some notations in order to be consistent with Peschel. We expand the exponential term, so that the wavefunction becomes

$$\Psi(\mathbf{x}) = C \exp\left(-\frac{1}{2}\sum_{ij} A_{ij} x_i x_j\right) \tag{20}$$

the coupling matrix A can also be expanded by normal modes. Note that $\phi_q \in col(U),\ q = 1, \ldots, N$ are the set of normal basis, A can be written as

$$A_{ij} = \sum_{q=1}^{N} \omega_q \phi_q(i)\phi_q(j) \tag{21}$$

where $\omega_q \in \sqrt{K_D}$. Then the full density matrix is

$$\rho(\mathbf{x}, \mathbf{x}') = \Psi(\mathbf{x})\Psi^*(\mathbf{x}') \propto \exp\left\{-\frac{1}{2}\sum_{ij} A_{ij}(x_i x_j + x_i' x_j')\right\} \tag{22}$$

To get the reduced density matrix ρ_l of a single l-th oscillator we calculate the following:

$$\rho_l(x_l, x_l') = \int \Big(\prod_{i\neq l} dx_i\Big) \Psi(x_1, \ldots, x_l, \ldots, x_N)\Psi^*(x_1, \ldots, x_l', \ldots, x_N) \tag{23}$$

where we set $x_i = x_i'$ if $i \neq l$. With this restriction and noting that A is symmetric, the full density matrix becomes

$$\rho(x_1, \ldots x_l, \ldots, x_N, x_1, \ldots x_l', \ldots, x_N) = C \exp\left\{-\sum_{i,j\neq l} A_{ij} x_i x_j - \sum_{j\neq l} A_{lj} x_j (x_l + x_l') - A_{ll}(x_l^2 + x_l'^2)\right\} \tag{24}$$