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1989 J. Phys.: Condens. Matter 1 8829

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Supersymmetric method for determining the vibrational frequency spectra of disordered crystals

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Received 8 March 1989, in final form 30 May 1989

Abstract. By using a supersymmetric functional integral formalism, the vibrational frequency spectrum of a one-dimensional monatomic linear-chain crystal in the presence of force constant disorder is calculated exactly in the continuum limit. More general disordered problems in one-dimensional vibrational systems can also be dealt with exactly using the same method.

1. Introduction

The problem of impurities in crystals has been attracting attention since the early 1950s [1–4]. There are a large number of publications in the literature investigating how the impurities affect the vibrational spectra of crystals [5–20]. It is well known that both electronic and vibrational problems can be treated in similar ways. For example, the average *t*-matrix method and coherent potential approximation have been used extensively to find either the electronic density of states or the vibrational frequency spectra [8, 9].

The most common types of disorder in electronic systems are site (diagonal) and bond (off-diagonal) disorder, where site disorder physically arises from, for instance, randomly distributed external charges while bond disorder comes from topologically disordered bond defects in the systems. Correspondingly, we also have two types of disorder in phonon systems, namely, mass and force constant disorder, respectively. The mass disorder is diagonal, hence it corresponds to the site disorder in electronic systems, while the force constant disorder corresponds to bond disorder.

For the electronic systems, due to the stochasticity of the Schrödinger equation describing electrons moving in a random potential, some of the problems (with Gaussian or Poisson random potentials) can be solved exactly in one dimension using classical methods that solve the Fokker–Planck equation and the recent supersymmetric functional integral formalism [4, 21, 22]. For phonon systems with either mass or force constant disorder, most of the theoretical investigations [10–15] have confined themselves to either single-site approximation theories or arbitrary concentration using various computational methods, for instance the equation-of-motion method [16] or the recursion method [17, 18, 19]. There has been so far no exact theory reported for calculating analytically arbitrary impurity concentrations in phonon systems to the author's knowledge.

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However, the supersymmetric functional integral formalism provides a useful method to average over the random disorder, hence it is an ideal candidate to investigate the phonon disorder problem. The traditional replica method fails to give correct results in some cases because the procedure whereby the replica index $n \rightarrow 0$ is mathematically unjustifiable (see [23]); the supersymmetry method, however, does not require this procedure. In [23], the authors studied the $\langle GG \rangle$ correlator of a typical problem for which the exact results are known but when the replica method is applied to either the bosonic or the fermionic manifold both results are incorrect unless one adopts the supersymmetric approach. Nonetheless, as far as the single-particle Green function $\langle G \rangle$ is concerned, no work has been reported where the replica results are different from those of the supersymmetric approach. In this paper, we employ a supersymmetric functional integral formalism and introduce superfields to deal with the disorder averaging prior to any other calculations. As a result, a problem of force constant disorder in phonon systems can be mapped to a problem of an electron moving in an effective random potential in the continuum limit of the supersymmetric functional integral formalism. It follows that one can obtain exact results for the vibrational frequency spectrum as in the cases of the electronic systems studied in [4, 21] and [22].

Unfortunately, for the problem of mass disorder in phonon systems, there is a non-trivial average one has to perform, namely, the average over $\langle \exp(\sum_l 1/M(l)) \rangle$, where $1/M(l)$ is the disordered mass term in the usual Lagrangian of phonon systems. It is hard to perform the average even for the simplest Gaussian-distributed random mass disorder because the random variables are in the denominator. One has to devise a more sophisticated method to deal with this average in order to obtain exact results; this is currently under investigation and the results will be published in a subsequent paper.

This paper is organised as follows: we introduce the general supersymmetric functional integral formalism and specify the random disordered lattice model in §2, give analysis and results in §3 and conclusions in §4.

2. Supersymmetric functional integral formalism

The model Lagrangian density we chose is the general one-dimensional linear chain with only nearest-neighbour interaction being considered (see [24]); it reads

$$L = \sum_l \lambda a \left(\frac{(\dot{\phi}(l))^2}{2} - \frac{c^2}{2a^2} (\phi(l+1) - \phi(l))^2 - \omega_0^2 V(\phi) \right) \quad (2.1)$$

where ϕ is displacement field and λa sets up the energy scale, i.e. λ is in units of (energy * (time)²)/length, c^2 is the scaled force constant in units of (length)²/(time)², a is the lattice constant and $V(\phi)$ is the so called cage potential which we will explain later. We take $V = \phi^2/2$ and ω_0^2 is the strength of the potential. The first term is the usual kinetic energy term and the second can be converted to the dynamical matrix for the one-dimensional monatomic linear chain straightforwardly.

The vibrational frequency distribution function is given by

$$G(\omega^2) = \frac{1}{\pi \lambda a N} \lim_{\epsilon \rightarrow 0^+} \text{Im} \sum_n \frac{1}{\omega^2 - \omega_n^2 - i\epsilon} \quad (2.2)$$

with the sum on n over all modes, where λa is introduced for later convenience.

In the presence of disorder, the frequencies $\{\omega_n\}$ cannot be found in general. Fortunately, the supersymmetry method allows us to construct a simple procedure for calculating the *average* frequency spectrum $\langle G(\omega^2) \rangle$ if the statistical properties of the disorder are known and the disorder is of a simple enough type.

Using a treatment similar to [21, 22] and [25], we introduce the Grassmann field χ , where the Grassmannian integrations are defined as

$$\int d\chi d\chi^* (1, \chi, \chi^*, \chi^* \chi) = (0, 0, 0, 1) \tag{2.3}$$

and the most useful integral formula

$$\int \prod_1^N (d\chi_a d\chi_a^*) \exp\left(-\sum_{a,b} \chi_a^* M_{ab} \chi_b\right) = \det \mathbf{M}. \tag{2.4}$$

We also note that the familiar conventional Gaussian integral is

$$\int \prod_1^N \frac{dS_a dS_a^*}{\pi} \exp\left(-\sum_{a,b} S_a^* M_{ab} S_b\right) = \frac{1}{\det \mathbf{M}}. \tag{2.5}$$

So using the supersymmetric integral, we can write

$$G(\omega^2) = \frac{1}{\pi N} \lim_{\epsilon \rightarrow 0^-} \text{Im} \sum_n G_n(\omega^2) \tag{2.6}$$

with

$$G_n(\omega^2) = -i \int \Phi_{\alpha n} \Phi_{\alpha n}^\dagger \exp[-i\Phi_n^\dagger \lambda a(\omega^2 - \omega_n^2 - i\epsilon)\Phi_n] d\Phi_n^* d\Phi_n \tag{2.7}$$

where Φ_n is a supervector with two components

$$\Phi_n = \begin{pmatrix} \chi_n \\ S_n \end{pmatrix}. \tag{2.8}$$

$\{\chi_n\}$ are anticommuting Grassmann variables and $\{S_n\}$ are commuting variables. The index α denotes either of the two components of the supervector. It is clear that the Grassmann field χ introduced here plays the role of exponentiating the frequency squared denominator, which will make the averaging over disorder easier.

In order to incorporate the discrete nature of the lattice model, we need to define the lattice superfield $\Phi(l)$ by

$$\Phi(l) = \sum_n \Phi_n \xi_n(l) \quad \Phi^\dagger(l) = \sum_n \Phi_n^\dagger \xi_n^*(l) \tag{2.9}$$

where $\{\xi_n(l)\}$ are eigenvectors of the dynamical matrix for the vibrational problem:

$$\mathbf{D}\xi_n = \omega_n^2 \xi_n. \tag{2.10}$$

The inversion of equations (2.9) gives

$$\Phi_n = \sum_l \xi_n^*(l) \Phi(l) \quad \Phi_n^\dagger = \sum_l \xi_n(l) \Phi^\dagger(l). \quad (2.11)$$

Equation (2.7) can be rewritten as

$$G_n(\omega^2) = -i \int \Phi_{z_n} \Phi_{z_n}^\dagger \exp \left(-i \sum_m \Phi_m^\dagger \lambda a (\omega^2 - \omega_m^2 - i\epsilon) \Phi_m \right) d\Phi_1^* d\Phi_1 \dots d\Phi_N^* d\Phi_N \quad (2.12)$$

since we are simply including several integrations as factors, each of which is unity (see [21] for details):

$$1 = \int \exp [-i \Phi_j^\dagger \lambda a (\omega^2 - \omega_j^2 - i\epsilon) \Phi_j] d\Phi_j^* d\Phi_j. \quad (2.13)$$

In order to compute the $G(\omega^2)$ one has to transform to the site representation; we have

$$\begin{aligned} \sum_n \Phi_n^\dagger \lambda a (\omega^2 - \omega_n^2 - i\epsilon) \Phi_n &= \sum_l \sum_{l'} \Phi^\dagger(l) \lambda a [(\omega^2 - i\epsilon) \delta_{ll'} - D(l'l')] \Phi(l') \\ &= \Phi^\dagger \lambda a [(\omega^2 - i\epsilon) \mathbf{I} - \mathbf{D}] \Phi \end{aligned} \quad (2.14)$$

where

$$\Phi = \begin{pmatrix} \Phi(1) \\ \Phi(2) \\ \vdots \\ \Phi(N) \end{pmatrix} \quad \Phi^\dagger = (\Phi^\dagger(1), \Phi^\dagger(2), \dots, \Phi^\dagger(N)) \quad (2.15)$$

and use has been made of the completeness and equation of motion of ξ_m , i.e. $\sum_m \xi_m^*(l') \xi_m(l'') = \delta_{l'l''}$ and equation (2.10).

The final form of the spectrum function is

$$\begin{aligned} G(\omega^2) &= \sum_l \frac{1}{\pi N} \lim_{\epsilon \rightarrow 0^+} \text{Im} \left(-i \int \prod_j d\Phi^*(j) d\Phi(j) \Phi(l) \Phi^\dagger(l) \right. \\ &\quad \left. \times \exp [-i \Phi^\dagger \lambda a ((\omega^2 - i\epsilon) \mathbf{I} - \mathbf{D}) \Phi] \right) \end{aligned} \quad (2.16)$$

where $\mathbf{D} = -(c^2/2a^2)\Psi + \omega_0^2 \mathbf{I}$ can be derived straightforwardly from the Lagrangian equation (2.1) with Ψ the standard force constant matrix.

Now we are in a position to do the average over the disorder, and thus we need to specify the type of disorder. The simplest type of disorder is 'force constant' disorder [1, 15, 17]; it can arise for example from bond defects or topological disorder in crystals. Of course, realistically, mass disorder exists as well. For simplicity and mathematical explicitness we treat only force constant disorder in this paper and leave the non-trivial mass disorder case to a forthcoming paper.

We consider that the dynamical matrix \mathbf{D} consists of a ‘pure’ part and a part due to disorder, i.e. [9]

$$D(l'l') = -D_0(l'l') + \omega_0^2 \delta_{ll'} + D_{\text{ran}}(l'l') = -\frac{c_0^2(l'l')}{2a^2} + \omega_0^2 \delta_{ll'} + \frac{c_{\text{ran}}^2(l'l')}{2a^2}$$

where the first two terms are the unperturbed force constant, the third is the random part and all the masses are the same. We assume a Gaussian random distribution such that the Gaussian δ -correlation law is satisfied, i.e. $\langle c_{\text{ran}}^2(l'l')c_{\text{ran}}^2(l''l''') \rangle = \gamma \delta_{ll',l''l'''}$, $\langle c_{\text{ran}}^2 \rangle = 0$, where γ denotes the strength of the force constant disorder. The Gaussian distribution law can be derived quite naturally in most physical systems provided the system is large enough that the central-limit theorem can be applied and the disorder is not very strong (see [26]). One can surely take a Poisson distribution (and other types as well) in this supersymmetric functional integral formalism; however, more numerical calculations will be involved to compute the vibrational frequency spectrum and one has difficulty obtaining analytic and closed form solutions even in the continuum limit.

Due to the Gaussian distribution, we can easily perform the functional integrations to obtain

$$\left\langle \exp \left(-i \sum_{l'l''} \Phi^\dagger(l) D_{\text{ran}}(l'l'') \Phi(l'') \right) \right\rangle = \exp \left(- \sum_{l'l''} f(l'l'') \right) \tag{2.17}$$

so that equation (2.16) becomes

$$G(\omega^2) = \frac{1}{\pi N} \lim_{\epsilon \rightarrow 0^+} \text{Im} \left[-i \sum_l \int \mathbf{D} \Phi^* \mathbf{D} \Phi \Phi(l) \Phi^\dagger(l) \right. \\ \left. \times \exp \left(-i \lambda a \sum_{l'l''} \Phi^\dagger(l) [(\omega^2 - \omega_0^2 - i\epsilon) \delta_{ll'} + D_0(l'l'')] \Phi(l'') - \sum_{l'l''} f(l'l'') \right) \right]. \tag{2.18}$$

with

$$f(l'l') = \left(\frac{\lambda^2 \gamma}{8a^2} \right) [(\Phi^*(l+1)\Phi(l))^2 + 4(\Phi^*(l)\Phi(l))^2 + (\Phi^*(l)\Phi(l-1))^2]$$

denoting the average over the disorder (see appendix 1 for details). It is clearly a non-local and non-linear term which precludes the possibility of getting an exact and closed form solution for the vibrational frequency spectrum. However, to understand low-frequency behaviour of the vibrational systems one only needs to study the long-wavelength limit, i.e. $a \rightarrow 0$, the continuum limit. In that limit we will have a local Φ^4 Lagrangian. To make this apparent, we expand $\Phi(l+1)$, $\Phi(l-1)$ around $\Phi(l)$, and we find that terms of first order in a are cancelled and the next non-vanishing terms are $O(a^2)$; it follows that we can neglect them safely in the continuum limit.

3. Results and discussion

From equation (2.18) and after taking the continuum limit our effective Lagrangian can be written as

$$L_{\text{eff}} = \sum_l i \lambda a \omega_0^2 \left[\Phi^\dagger(l) \left(\frac{\omega^2}{\omega_0^2} - 1 - i\epsilon \right) \Phi(l) + \frac{c_0^2}{2\omega_0^2 a^2} |\Phi^*(l+1) - \Phi(l)|^2 \right. \\ \left. - i \frac{3\lambda\gamma}{4a^3 \omega_0^2} (\Phi^*(l)\Phi(l))^2 \right]. \tag{3.1}$$

In order to make a dimensionless Lagrangian we note that Φ fields have units of $1/\text{energy}^{1/2} = 1/(\lambda c_0^2/a)^{1/2}$ and $\gamma = \bar{\gamma} c_0^4$. Due to the one dimensionality, one can use the transfer operator method [27, 28] to solve the problem exactly. We first set the arguments l of the Φ fields in the integrand of equation (2.18) to be different, say l and l' for convenience, and we will set $l = l'$ later on when we study the vibrational frequency spectrum which requires $l = l'$ only. We have

$$G(\omega^2) = \frac{1}{\pi N} \sum_l \lim_{\epsilon \rightarrow 0^-} \text{Im} \left(i \int \Gamma(0, l; R^0, R) \chi(l) \right. \\ \left. \times \Gamma(l, l'; R, R') \chi^*(l') \Gamma(l', n; R', R^n) dR^0 dR dR' \right) \quad (3.2)$$

where

$$R \equiv \{\chi, \chi^*, S, S^*\} \quad \text{and} \quad dR \equiv \frac{1}{\pi} d\chi^* d\chi dS^* dS. \quad (3.3)$$

n labels the last site which will be infinity when we take the thermodynamic limit and na gives the total length of the crystal. The kernel Γ in the above equation satisfies the following effective Schrödinger equation when passing to the continuum limit, i.e. $a \rightarrow 0$ (see appendix 2 for details),

$$\left(-\frac{\partial}{\partial x} + \mathcal{H}(R) \right) \Gamma(x, x'; R, R') = \delta(x - x') \delta(R - R') \quad (3.4)$$

where

$$\mathcal{H} = -\frac{2}{\mu} \left(\frac{\partial^2}{\partial S^* \partial S} + \frac{\partial^2}{\partial \chi^* \partial \chi} \right) + \mu(\bar{\omega}^2 - \bar{\omega}_0^2)(|S|^2 + |\chi|^2) + \frac{3\bar{\gamma}}{4} (|S|^2 + |\chi|^2)^2 \quad (3.5)$$

with all the fields dimensionless and $\bar{\omega} = \omega/\Omega_0$, $\bar{\omega}_0 = \omega_0/\Omega_0$, $\Omega_0 = (c_0^2/a_0^2)^{1/2}$, and where $\bar{\gamma}$ is also dimensionless as defined before. The δ -functions are defined in the usual sense, $|\chi|^2 = \chi^* \chi$ and μ will be set equal to i later on. Following the same procedures as in [21, 22, 29], we obtain the phonon frequency spectrum per unit mode and per site $G(\bar{\omega}^2)$ in terms of Airy functions [30]

$$G(\bar{\omega}^2) = \frac{4}{\pi^2 (3\bar{\gamma})^{1/3}} \frac{\text{Ai}'(z)\text{Ai}(z) + \text{Bi}'(z)\text{Bi}(z)}{[\text{Ai}^2(z) + \text{Bi}^2(z)]^2} \quad (3.6)$$

where $z = -(\bar{\omega}^2 - \bar{\omega}_0^2)/(3\bar{\gamma})^{2/3}$. The results are quite similar to that obtained for disordered electronic systems, e.g. [4, 22]. The similarity tells us that in one-dimensional systems with Gaussian-distributed random disorder, no matter whether the systems are vibrational or electronic, Airy functions play important roles in describing the density of states of the systems. Both exponential band tails and the characteristic $1/\omega$ law for 1D phonon systems, $1/(E^2 - E_0^2)^{1/2}$ law for 1D electronic systems within the band can be obtained easily by taking asymptotic expansions of the Airy functions. The nice properties of the Airy functions exclude singularities and exact zeros in the density of

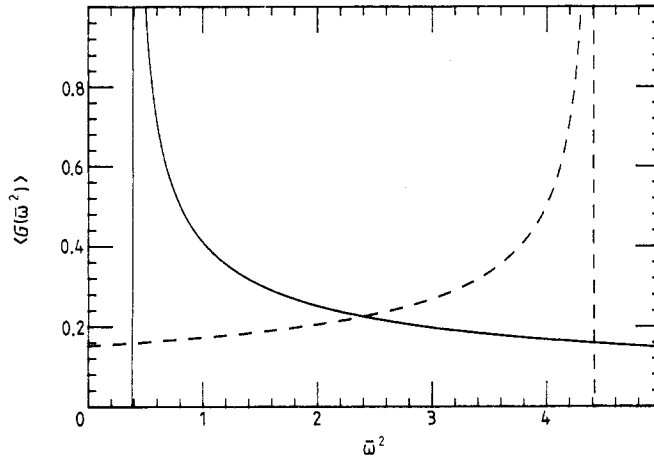


Figure 1. $G(\bar{\omega}^2)$ plotted against $\bar{\omega}^2$ with $\bar{\omega}_0^2 = 0.4$, where $\bar{\gamma} \rightarrow 0$ ($= 0.0001$) for both full curve and broken curve (effective modulus method) results. The $1/\bar{\omega}$ tails are purely consequences of taking the continuum limit; they should be discarded for the discrete model and the full curve and broken curve results should be smoothly connected at intermediate $\bar{\omega}$.

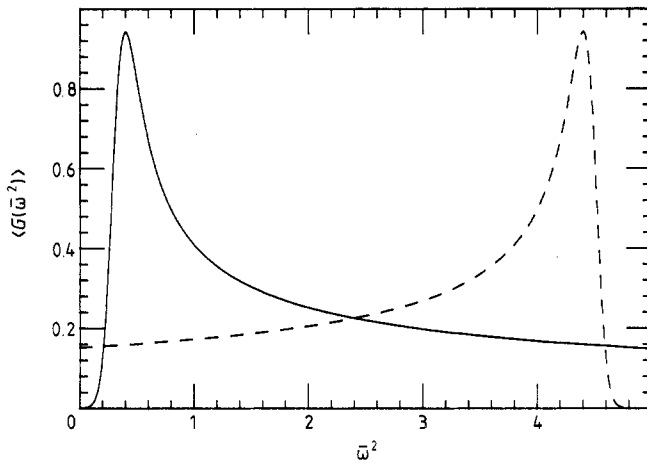


Figure 2. $G(\bar{\omega}^2)$ plotted against $\bar{\omega}^2$ with $\bar{\omega}_0^2 = 0.4$, where $\bar{\gamma} = 0.01$ for both full curve and broken curve results.

states, in general, which ties in with general discussions of one-dimensional disordered systems (except some special points in some special systems [31, 32]).

In the figures we plot the vibrational frequency spectrum $G(\bar{\omega}^2)$ with different values of $\bar{\gamma}$. When $\bar{\gamma} \rightarrow 0$ which is the clean limit, our result reproduces the unperturbed phonon density of states, exactly as shown in figure 1. It has $1/\bar{\omega}$ singularities near the zero-frequency (full curve) and Brillouin zone boundary (broken curve, which is again an exact result obtained by using the effective modulus method [33] with the continuum limit taken near the BZ boundary). For finite but small $\bar{\gamma}$, the $1/\bar{\omega}$ singularity disappears and a peak is found corresponding to the effects of the random force constant. A very sharp exponential band tail can be seen clearly in figure 2 and has the form

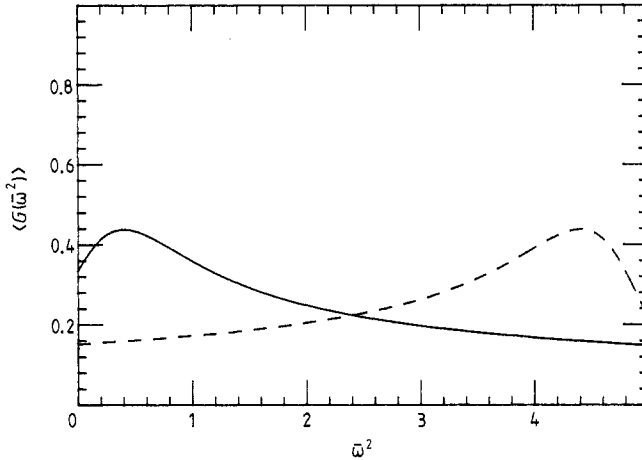


Figure 3. $G(\bar{\omega}^2)$ plotted against $\bar{\omega}^2$ with $\bar{\omega}_0^2 = 0.4$, where $\bar{\gamma} = 0.1$ for both full curve and broken curve results.

$\sim \exp[-(\bar{\omega}^2 - \bar{\omega}_{\text{BZB}}^2)^{3/2}]$, which is the first analytic expression for the band tails in disordered phonon systems. The $1/\bar{\omega}$ tails ($\bar{\omega} \gg 0$ for full curve results; $\bar{\omega} \ll \bar{\omega}_{\text{BZB}}$ for broken curve results) are purely consequences of taking the continuum limit, which should be discarded for real discrete lattice problems and, furthermore, the full curve results and broken curve results should connect smoothly at an intermediate range of $\bar{\omega}$. However, this definitely cannot be done within the continuum model. In order to describe the correct behaviour of the density of states in the intermediate range of ω , one either has to do *ab initio* simulations for a real discrete lattice model or take into account higher-order discreteness corrections that the continuum model left out and which will not be discussed in this paper.

4. Concluding remarks

By employing the supersymmetric functional integral formalism we have obtained an exact and analytic expression for the vibrational frequency spectrum of a one-dimensional monatomic linear chain with force constant disorder, in the continuum limit. The exact analytical expression can be easily analysed to compare with results from other calculations in different regimes of impurity concentrations. We note that this is only a pure theoretical model calculation. For more realistic 1D lattice systems one has to consider higher-order discreteness corrections. Nonetheless, the approach provided a starting point for more realistic calculations without having to rely too heavily on numerical simulations.

We also note that the cage potential V stabilises the system and makes the finite temperature displacement field averaging be finite; without this stabilising potential the thermal average $\langle x \rangle_T = \infty$. The other point we want to make is that due to the Gaussian distribution law, which has a non-zero probability for disordered force constants to reach very large negative values, the system generates some non-physical (negative frequency) vibrational modes. However, they are exponentially small in the density of states for weak disorder. Instead, one needs to choose other probability

distribution laws in more realistic models, such as the Poisson, to avoid this large negative force constant instability.

As a consequence, one can apply this method to a series of problems which can be effectively mapped to a disordered harmonic linear-chain model to find out their vibrational frequency spectra analytically and based on that one can compute other interesting quantities such as the root mean displacement and the momentum. More interestingly, the experimentally related quantities for vibrational systems are the static and dynamic structural factors (Fourier transformed) which may also be found by using the SUSY method. This method also works for higher-dimensional problems [25, 34]; however, there is no general guide to solving arbitrary n -dimensional supersymmetric functional integrations exactly so far.

Acknowledgments

The author would like to thank both S E Trullinger and A R Bishop for suggesting the problem and R M Stratt for helpful discussions.

Appendix 1

In this appendix we will give the details of how to average over the random disorder potential by using the SUSY functional integral formalism.

We need to perform the average

$$I = \left\langle \exp \left(-i \sum_{l'} \Phi^\dagger(l) D_{\text{ran}}(l'l') \Phi(l') \right) \right\rangle \quad (\text{A1.1})$$

where the D_{ran} matrix is defined as

$$D_{\text{ran}}(l'l') = \frac{\lambda}{2a} \begin{pmatrix} 2\delta K_{11} & -\delta K_{1,2} & 0 & 0 & 0 & \dots & 0 \\ -\delta K_{2,1} & 2\delta K_{22} & -\delta K_{2,3} & 0 & 0 & \dots & 0 \\ 0 & -\delta K_{3,2} & 2\delta K_{33} & -\delta K_{3,4} & 0 & \dots & 0 \\ & & & \vdots & & & \\ 0 & 0 & \dots & 0 & 0 & -\delta K_{n,n-1} & 2\delta K_{nn} \end{pmatrix}$$

with $\delta K = c_{\text{ran}}^2$ denoting the random part of the force constant. For the Gaussian case we have, in general,

$$\begin{aligned} \langle \delta K_{l_1} \delta K_{l_2} \dots \delta K_{l_{2n+1}} \rangle &= 0 \\ \langle \delta K_{l_1} \delta K_{l_2} \dots \delta K_{l_{2n}} \rangle &= \sum_{(l_1 \dots l_{2n})} \gamma^n \delta_{l_1 l_2} \dots \delta_{l_{2n-1} l_{2n}} \end{aligned} \quad (\text{A1.2})$$

where the summation extends over all possible partitions of the $2n$ indices $(1, 2, \dots, 2n)$, into n parts $(l_1, l_2) \dots (l_{2n-1}, l_{2n})$ and for different sites the average is uncorrelated. For a one-dimensional monatomic chain, we have

$$I = \left\langle \exp \left(-i \sum_l \frac{\lambda}{2a} (\Phi^\dagger(l+1) K_{l+1} \Phi(l) - 2\Phi^\dagger K_l \Phi(l) + \Phi^\dagger(l) K_{l-1} \Phi(l-1)) \right) \right\rangle. \quad (\text{A1.3})$$

For example, the second term gives:

$$I_2 = \sum_{\nu=0}^{\infty} \frac{(-i\lambda/a)^\nu}{(\nu)!} \langle \delta K_{l_1+1} \delta K_{l_2+1} \dots \delta K_{l_\nu+1} \rangle \times \sum_{l_1} \Phi^*(l_1+1)\Phi(l_1) \dots \sum_{l_\nu} \Phi^*(l_\nu+1)\Phi(l_\nu) \tag{A1.4}$$

using equation (A1.2) we have

$$I_2 = \sum_{\mu=0}^{\infty} \frac{(i\lambda/a)^{2\mu}}{(2\mu)!} \gamma^\mu (2\mu-1)!! \left| \sum_l (\Phi^*(l+1)\Phi(l))^2 \right|^\mu = \exp \left[- \left(\frac{\gamma(\lambda)^2}{2a^2} \right) \sum_l (\Phi^*(l+1)\Phi(l))^2 \right] \tag{A1.5}$$

where the identity $(2\mu)! = 2^\mu(2\mu-1)!!\mu!$ has been used. The other two terms are similar. Adding them together we get

$$I = \exp \left[- \left(\frac{\gamma(\lambda)^2}{8a^2} \right) [(\Phi^*(l+1)\Phi(l))^2 + 4(\Phi^*(l)\Phi(l))^2 + (\Phi^*(l)\Phi(l-1))^2] \right]. \tag{A1.6}$$

Appendix 2

In this appendix we will show how to start from the discrete formalism and then pass to the continuum limit to get equation (3.4).

From equation (3.1) the first and third terms are easily converted to the continuum version by considering that $\sum a \rightarrow \int dx$ and $\Phi(l+1) \rightarrow \Phi(x+a)$ where a is the lattice constant that will be equal to dx at the continuum limit.

As usual, we use the transfer operator method (see [28]) and introduce a delta function as a bilinear expansion in a set of complete orthonormal functions $\{v_n(\Phi)\}$:

$$\delta(\Phi_{N+1} - \Phi_1) = \sum_n v_n^*(\Phi_{N+1})v_n(\Phi_1) \tag{A2.1}$$

$$\delta(\Phi_{N+1}^* - \Phi_1^*) = \sum_n v_n^*(\Phi_1^*)v_n(\Phi_{N+1}^*) \tag{A2.2}$$

where the particular set of functions $\{v_n^*v_n\}$ is conveniently chosen to satisfy the transfer integral equation

$$\int_{-\infty}^{+\infty} d\Phi(l) d\Phi^*(l) \exp[-h(\Phi^*(l+1), \Phi(l))] v_n^*(\Phi^*(l))v_n(\Phi(l)) = \exp(-E_n\lambda a)v_n^*(\Phi^*(l+1))v_n(\Phi(l+1)) \tag{A2.3}$$

where E_n is the associated eigenvalue of the transfer integral equation

$$h = \frac{\mu\lambda ac_0^2}{2} \left(\frac{\Phi^*(l+1) - \Phi(l)}{a} \right)^2 + \frac{\lambda ac_0^2}{2} [v(\Phi^*(l+1)\Phi(l+1)) + v(\Phi^*(l)\Phi(l))] \tag{A2.4}$$

and

$$v(\Phi^* \Phi) = \mu \Phi^\dagger \left(\frac{\omega^2}{\omega_0^2} - 1 - i\epsilon \right) \Phi + \frac{3\gamma\lambda}{4a^3\omega_0^2} (\Phi^* \Phi)^2 \quad (\text{A2.5})$$

is the effective potential, μ will be set equal to i later on. We split equation (A2.4) ($v(l) = \frac{1}{2}[v(l+1) + v(l)]$) just for later convenience since the system is symmetric on exchanging $l+1$ and l . Now set

$$\bar{v}_n^*(\Phi^* \Phi) \bar{v}_n(\Phi^* \Phi) = \exp(-\frac{1}{2} a \lambda \omega_0^2 v(\Phi^* \Phi)) v_n^*(\Phi^* \Phi) v_n(\Phi^* \Phi) \quad (\text{A2.6})$$

and Taylor expand the $\bar{v}_n(\Phi(l))$ functions about $\bar{v}_n(\Phi(l+1))$ and do the Gaussian integrations with respect to the $\Phi(l)$ fields, then re-sum the results; we end up with

$$\exp\left(\frac{2a}{\lambda\mu c_0^2} \frac{d^2}{d\Phi^* d\Phi}\right) \bar{v}^* \bar{v} = \exp\{-\lambda a \omega_0^2 [E_n - v_0 - v(\Phi^* \Phi)]\} \bar{v}^* \bar{v}. \quad (\text{A2.7})$$

We note that $v_0 = (1/\lambda a \omega_0^2) \ln(\lambda c_0^2 \omega_0^2 / a)$ is a constant which can be absorbed into the normalisation constant (see [26] for details); it can also be treated as an energy minimum (see [35]) in the discrete lattice problems, but when we absorb it into the normalisation constant we actually have this energy minimum as zero.

Using the commutator identity

$$e^B e^A e^B = e^{A+2B+(1/3!)[A+B, [A,B]]+\dots} \quad (\text{A2.8})$$

and substituting equation (A2.6) into equation (A2.7), we found that the non-zero order correction is of the order of a^2/l_0^2 (where $l_0^2 = c_0^2/\omega_0^2$) and can thus be neglected in the first-order approximation, i.e. the continuum limit, as long as $a \ll l_0$. Putting all the dimensionless quantities as defined before into equation (A2.7) we finally obtain equation (3.5).

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