Physics 525, Condensed Matter

Homework 6

Due Tuesday, 21st November 2006

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Problem 1: Thermal Expansion of a One-Dimensional Crystal via Anharmonicities

Consider a simple one-dimensional crystal lattice with nearest-neighbour interaction potential

$$\varphi(y) = \frac{K}{2}y^2 - gy^3, \tag{1.1}$$

where $y = x_{i+1} - x_i - a_0$ and g is small; a is the lattice spacing. For $g = 0$ and at zero external pressure the lattice spacing $a = a_0$ and the probability distribution of y due to zero-point thermal phonons is Gaußian with root-mean-square $\sigma(T)$ at temperature T; we are to treat $\sigma(T)$ as a known function.

By perturbatively adding the effects of the cubic anharmonicity, we are to determine the equilibrium lattice spacing a to leading order in g. We should use this to express the thermal expansion coefficient in terms of the specific heat at $g = 0$ and other parameters in the problem. We should estimate the magnitude of g for which this approximation is valid.

A lot of physics intuition leads us to expect that to leading order in g the equilibrium anharmonic lattice can be viewed as a harmonic system with modified equilibrium displacements[1]. The heuristic picture we have in mind is this: if g is turned on slowly, the lattice spacing may change reaching some new equilibrium value; but the fluctuations about this new lattice spacing should still be roughly Gaußian—and the widths of the distributions shouldn't know anything about g to leading order[2].

Because the harmonic system amounts to a collection of N independent oscillators (each with the same Gaußian normal distribution) the entropy of the system is simply the sum of the entropies of each. This has nothing to do with the lattice spacing, so if we are allowed to view the perturbed system as identical to the original system with an 'expanded' lattice spacing, then the entropy should not be changed. We expect this argument to hold to leading order in g. This implies that the entropy is independent of g to leading order—and therefore minimization of the free energy is equivalent to minimization of the energy u.

Using our reasoning above, we see that the expectation value of the total energy per lattice site u should therefore be given by[3]

$$\langle u\rangle = u_0 + \frac{1}{\sigma(T)\sqrt{2\pi}}\int_{-\infty}^{\infty} dy \;\; \exp\left\{-\frac{(y-\delta a)^2}{2\sigma^2(T)}\right\}\left(\frac{K}{2}y^2 - gy^3\right) + \mathcal{O}(g^2), \tag{1.2}$$

$$= u_0 + \frac{K}{2}\sigma^2(T) - 3g\sigma^2(T)\delta a + \frac{K}{2}\delta a^2 - g\delta a^3 + \mathcal{O}(g^2). \tag{1.3}$$

Notice that the expression above makes sense when $g = 0$: then equation (1.3) reads $\langle u\rangle = u_0 + \frac{K}{2}\sigma^2 = u_0 + \frac{K}{2}\langle y^2\rangle$ when the displacement is unchanged, i.e. $\delta a = 0$—we will show presently that $g = 0$ implies $\delta a = 0$.

To find the modified lattice spacing for non-vanishing g, we should minimize the total energy (1.3) with respect to δa. This can be done by inspection. We find

$$K\delta a - 3g\delta a^2 - 3g\sigma^2(T) = 0, \tag{1.4}$$

which implies that

$$\delta a = \frac{3g}{K}\left(\sigma^2 + \delta a^2\right) = \frac{3g}{K}\sigma^2 + \mathcal{O}(g^2). \tag{1.5}$$

To check consistency, we observe that $g = 0$ implies δa vanishes.

[1] If we think in terms of Feynman diagrams, then it takes one factor of g to communicate the anharmonicity between neighbouring lattice sites, but at least two powers of g to communicate anharmonicity between two fluctuations; so to leading order in g, we expect the distributions to be offset, but otherwise unchanged.

[2] Note added in revisions: this is obvious from the fact that we're considering an adiabatic process.

[3] The 'higher order' terms in equation (1.2) arise from, e.g., non-Gaußianity in the structure of the fluctuations past leading order.

The thermal expansion coefficient is then seen to be[4]

$$\alpha \equiv \frac{1}{a_0+\delta a}\frac{d(\delta a)}{dT} = \frac{1}{a_0}\frac{6g}{K}\sigma\frac{d\sigma}{dT} + \mathcal{O}(g^2). \tag{1.6}$$

Setting $g \to 0$ in expression (1.3) we find the original thermal heat capacity to be

$$c_v = \frac{2}{a_0}K\sigma\frac{d\sigma}{dT}. \tag{1.7}$$

Therefore, we can write the thermal expansion coefficient α as

$$\therefore \alpha = \frac{3g}{K^2}c_v + \mathcal{O}(g^2). \tag{1.8}$$

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The leading order approximation in g is valid only when the anharmonic contribution to the potential is small compared to the harmonic contribution. Inserting our expression for δa into equation (1.3) we find that our condition is[5]

$$\begin{aligned} 3g\ \sigma^2\ \delta a + g\ \delta a^3 &< \frac{K}{2}(\sigma^2+\delta a^2); \\ \implies \quad \frac{3}{2}g\ \delta a\ \sigma^2 &< \frac{K}{2}\sigma^2; \\ \implies \quad g &< \frac{K^2}{9g\sigma^2}; \end{aligned}$$

and therefore our approximations are appropriate as long as

$$|g| < \frac{K}{3\sigma}. \tag{1.9}$$

Problem 2: Electrons in Two-Dimensions

Consider a two-dimensional gas of electrons (confined to, say, the xy-plane) subjected to a uniform magnetic field B in the positive $\hat{z}$ direction and a uniform electric field $\vec{E} = E\hat{x}$, giving rise to a two-dimensional potential $U(x,y) = eEx$.[6] We may assume for the sake of convenience that the system is of large length L in the $\hat{y}$-direction so that we may impose periodic boundary conditions in that direction.

a. We are to find all the single-electron eigenstates and their corresponding eigenenergies.

From our experience working with gauge fields, we know that to upgrade the Schrödinger equation for a free electron to one in a non-trivial gauge potential $A_\mu = (\varphi, -\vec{A})$[7],[8], all we must do is upgrade $\partial_\mu \mapsto \partial_\mu + i\frac{q}{\hbar}A_\mu$ everywhere. In our setup, the scalar potential $\varphi(x,y) = -Ex$ and we will choose the Lorentz gauge for the magnetic field so $\vec{A} = Bx\hat{y}$. This means that

$$\begin{aligned} \hat{H}\psi = i\hbar\partial_t\psi &= \frac{1}{2m}\left((-i\hbar\partial_x)^2 + (-i\hbar\partial_y)^2\right)\psi \\ \mapsto i\hbar\left(\partial_t - i\frac{e}{\hbar}(-Ex)\right)\psi &= \frac{1}{2m}\left[(-i\hbar\partial_x)^2 + \left(-i\hbar\left(\partial_y + i\frac{e}{\hbar}Bx\right)\right)^2\right]\psi, \\ \therefore i\hbar\partial_t\psi = \hat{H}\psi &= \frac{1}{2m}\left[-\hbar^2\partial_x^2 - \hbar^2\partial_y^2 - 2i\hbar eBx\partial_y + e^2B^2x^2\right]\psi + eEx\psi. \end{aligned} \tag{2.a.1}$$

[4]Notice that $\frac{1}{a_0+\delta a} = \frac{1}{a_0} + \mathcal{O}(\delta a)$—and that the part of $\mathcal{O}(\delta a)$ is over order g and so can be neglected when multiplying terms of order g.

[5]A quicker calculation, using equation (1.1), would give $g < \frac{K}{\sqrt{6}\sigma}$ which is a bit stronger than what we obtain above—but the difference is not very substantive.

[6]To avoid confusion—which is not easy to do in this problem—e will always be take to be the absolute value of the electron's charge. This ensures that the E-field points in the positive x-direction, but it forces us to systematically alter the equations copied in lecture (where 'e' was often used to denote the charge q).

[7]We are going to set $c = 1$ to avoid lots of confusion. If at the end units are desired, there is always a unique way of adding c to the expressions.

[8]However, I am quite sure that the spatial components of A_μ come with a minus sign: this important fact comes about via the metric. Many textbooks disappointingly do not clarify how all these signs work out. (Indeed, it is a common practice of field theory textbooks to define the gauge covariant derivative of QED oppositely to all other gauge fields so that a familiar minus sign is present for the electron.)

We may suppose that ψ is separable—specifically, of the form $\psi(x,y) = \widetilde{\varphi}(x)e^{-iky}$. Periodic boundary conditions of course require that $k \equiv k_n = \frac{2\pi n}{L}$ for some nonnegative integer n[9]. Inserting this into the Schrödinger equation (2.a.1), we find that

$$\hat{H}\varphi(x) = \left[-\frac{\hbar^2}{2m}\partial_x^2 + \frac{\hbar^2}{2m}k_n^2 - \frac{\hbar k_n eBx}{m} + \frac{e^2}{2m}B^2x^2 + eEx\right]\widetilde{\varphi}(x). \tag{2.a.2}$$

To make this conceptually easier, we should try as hard as we can to simplify the structure. Although not apparently obvious, it may prove useful to define the cyclotron frequency ω_c and magnetic length ℓ_B:

$$\omega_c \equiv \frac{eB}{m} \qquad \text{and} \qquad \ell_B^2 \equiv \frac{\hbar}{eB}. \tag{2.a.3}$$

Making use of these constants, we see that equation (2.a.2) becomes

$$\begin{aligned}
\hat{H}\varphi &= \left[-\frac{\hbar^2}{2m}\partial_x^2 + \frac{m\omega_c^2}{2}\ell_B^4 k_n^2 - m\omega_c^2\ell_B^2 k_n x + \frac{m\omega_c^2}{2}x^2 + eEx\right]\widetilde{\varphi}(x), \\
&= \left[-\frac{\hbar^2}{2m}\partial_x^2 + \frac{m\omega_c^2}{2}\left(x - k_n\ell_B^2 + \frac{E}{B\omega_c}\right)^2 + eE\left(k_n\ell_B^2 - \frac{E}{B\omega_c}\right) + \frac{m}{2}\left(\frac{E}{B}\right)^2\right]\widetilde{\varphi}(x), \\
&= \left[-\frac{\hbar^2}{2m}\partial_x^2 + \frac{m\omega_c^2}{2}\left(x - x_n\right)^2 + eEx_n + \frac{m}{2}\left(\frac{E}{B}\right)^2\right]\widetilde{\varphi}(x),
\end{aligned} \tag{2.a.4}$$

where in the last line we have introduced

$$x_n \equiv k_n\ell_B^2 - \frac{E}{B\omega_c}.$$

Notice that equation (2.a.4) is the Schrödinger equation for simple harmonic oscillator with a displaced origin and a 'lifted' energy:

$$\hat{H}\varphi(x) = \left[-\frac{\hbar^2}{2m}\partial_x^2 + \frac{m\omega_c^2}{2}\left(x - x_n\right)^2\right]\widetilde{\varphi}(x) + \left[eEx_n + \frac{m}{2}\left(\frac{E}{B}\right)^2\right]\widetilde{\varphi}(x), \tag{2.a.5}$$

$$= \left(m + \tfrac{1}{2}\right)\hbar\omega_c + eEx_n + \frac{m}{2}\left(\frac{E}{B}\right)^2. \tag{2.a.6}$$

If we let $\varphi_m(x)$ denote the canonical simple harmonic oscillator wave function at level m, then the eigenenergies (2.a.6) correspond to eigenfunctions

$$\psi_{m,n}(x) = \varphi_m(x - x_n)e^{-ik_n y} \tag{2.a.7}$$

where m labels the Landau level and n labels the $\hat{y}$-momentum.

Now, the $\varphi_m(x - x_n)$ are Hermite polynomials centred at x_n. For a sample with a finite width W in the $\hat{x}$-direction, it should be the case that x_n lies within the sample. This implies that

$$\frac{E}{B\omega_c} < k_n\ell_B^2 < W + \frac{E}{B\omega_c}. \tag{2.a.8}$$

Because this confines k_n to a (finite) range of positive values, this agrees with our choice of signs earlier.

[9] See the discussion following equation (2.a.7) for an explanation.

b. Using the wavefunctions found above, we are to determine the total current carried by each state and compare this to the classical result for a particle undergoing cyclotron motion in perpendicular E and B fields and to the result obtained by using the semiclassical velocity $\vec{v} = \frac{1}{\hbar}\frac{d\varepsilon}{d\vec{k}}$.

It is rather straight-forward to compute the current of the wave functions found above.

Indeed, using equation (2.a.7) we find for the $\hat{x}$-component of the current[10]

$$\begin{aligned}\vec{j}_x = -ev_x &= -\frac{e}{m}\mathfrak{Re}\left\{\psi^*_{m,n}\hat{\Pi}\psi_{m,n}\right\},\\ &= -\frac{e}{m}\mathfrak{Re}\left\{\varphi^*_m(x-x_n)e^{-ik_n y}(-i\hbar)\partial_x\varphi_m(x-x_n)e^{ik_n y}\right\},\\ &= 0\end{aligned}$$

because we can choose the simple harmonic oscillator wave functions $\varphi_m(x)$ to be real. The $\hat{y}$-component of the current is found similarly,

$$\vec{j}_y = -\frac{e}{m}\mathfrak{Re}\left\{\varphi^*_m(x-x_n)e^{ik_n y}\left(-i\hbar\partial_y + eBx\right)\varphi_m(x-x_n)e^{-ik_n y}\right\}, \tag{2.b.9}$$

$$= \frac{e}{m}\left(\hbar k_n - eBx\right)\varphi^2_m(x-x_n)\hat{y}. \tag{2.b.10}$$

Considering the range of k_n allowed, this seems to give a current in the $+\hat{y}$-direction, as we would expect. The minimum value of $k_n > \frac{Em}{B\hbar}$.

The classical solution to crossed electric and magnetic fields is of course a cycloid. Indeed, if we consider the trajectory of an individual electron classically, we find it to be

$$x(t) = \frac{E}{\omega_c B}\Big((\cos(\omega_c t) - 1), (\sin(\omega_c t) - \omega_c t)\Big), \tag{2.b.11}$$

which gives rise to a net current in the positive $\hat{y}$-direction

$$\vec{j} = -e\langle\dot{y}(t)\rangle = \frac{E}{B}\hat{y}. \tag{2.b.12}$$

Semiclassically, we take the derivative of the energy (2.a.6) with respect to $-k_n$ to obtain

$$\vec{j} = (-e)\frac{1}{\hbar}\frac{-\hbar E}{eB} = \frac{E}{B}\hat{y}. \tag{2.b.13}$$

[10]Recall that the gauge-covariant momentum operator $\Pi = -i\hbar\vec{\nabla} + \frac{e}{\hbar}\vec{A}$.