Wigner-distribution- and Green's-function approach to quantum corrections and implications for the melting temperature of two-dimensional Wigner crystals

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(Received 14 February 1985)

Quantum corrections to the behavior of a nearly classical system may be determined via the Green's-function formalism, or via the Wigner-distibution-function (WDF) method. Recently, it appeared that there is a serious discrepancy between the results obtained by these methods for the melting temperature of the two-dimensional Wigner crystal. We resolve this problem by showing that the "effective-potential" technique of implementing the WDF method is invalid, and we present a correct approach.

The two-dimensional electron lattice is a focus of continuing interest as a test of the Kosterlitz-Thouless-Nelson-Halperin-Young theory of melting.[1-3] In this case the essential parameter determining the melting temperature is μ, the shear modulus.[4,5] Owing to anharmonicity, the shear modulus itself displays a significant variation with temperature, and an accurate determination of the melting temperature must take account of this fact. The shear modulus is found from the long-wavelength dispersion relation for transverse phonons:

$$\omega^2(\mathbf{k},t)=\frac{\mu}{mn_s}k^2+O(k^4)\ , \tag{1}$$

where m is the electron mass and n_s is the areal density of electrons. To determine the temperature dependence of μ, one must therefore compute the frequency shift $\Delta_t(\mathbf{k})$ for a transverse phonon, due to anharmonicity. In general, $\Delta_t(\mathbf{k})$ includes corrections which manifest themselves in two ways: classical thermal corrections (terms $\sim T$, T^2, etc.), and terms $\sim\hbar^2$, $\hbar^4$, etc., which represent the effects of quantum fluctuations.

Morf[6] estimated thermal anharmonic corrections to the phonon spectrum in a Monte Carlo simulation. His result, which yields a melting temperature close to the experimental value,[7-10] was subsequently corroborated in a Green's-function[11,12] calculation of Fisher.[5] Both thermal and quantum corrections to the shear modulus were calculated by Chang and Maki,[13] who found good agreement with Fisher's result for thermal effects. Somewhat earlier, Fukuyama[14] proposed a method for calculating quantum (but not thermal) corrections to the phonon spectrum via an "effective potential" derived from the Wigner-distribution function (WDF). However, Chang and Maki note a substantial discrepancy between their result and Fukuyama's. Thus far, experiments on electrons at the liquid-helium surface have been confined to the low density, classical regime, but recently proposed experiments using thin He films[15] should provide an opportunity for the study of quantum effects. Here we show that the effective potential defined by Fukuyama *cannot* be used to derive the frequency shift due to quantum fluctuations, and that the method is, quite generally, invalid. In addition, we show that Green's-function and WDF calculations predict the same results for the frequency of an anharmonic oscillator. We thereby resolve the apparent conflict between Green's-function and WDF predictions for the melting temperature of the two-dimensional electron lattice.

The (unnormalized) density operator for a canonical ensemble at inverse temperature $\beta=1/kT$ is $\hat{\Omega}=e^{-\beta\hat{H}}$, where $\hat{H}$ is the n-particle Hamiltonian. The corresponding (unnormalized) WDF is[16,17]

$$\Omega(q_1,q_2,\ldots,q_n,p_1,p_2,\ldots,p_n)\equiv\int dy_1\int dy_2\cdots\int dy_n\,\langle q_1-y_1,q_2-y_2,\ldots,q_n-y_n|\hat{\Omega}|q_1+y_1,q_2+y_2,\ldots,q_n+y_n\rangle \times\exp\left[\frac{2i}{\hbar}(p_1\cdot y_1+p_2\cdot y_2+\cdots+p_n\cdot y_n\right]\ , \tag{2}$$

where q_i and p_i are coordinate and momentum vectors for the ith particle. [The range of integration in Eq. (2) and all subsequent formulas is from $-\infty$ to $+\infty$.] Ω may be obtained by solving the phase-space representation of the Bloch equation.[16,17] In terms of Ω, the ensemble average of any function $F(\hat{q}_1,\hat{q}_2,\ldots,\hat{q}_N)$ of coordinates is

$$\langle F\rangle=\frac{\mathrm{Tr}[F(\hat{q}_1,\hat{q}_2,\ldots,\hat{q}_n)\hat{\Omega}]}{\mathrm{Tr}[\hat{\Omega}]} =\frac{\int dp_1\int dp_2\cdots\int dp_n\int dq_1\int dq_2\cdots\int dq_n\,F(q_1,q_2,\ldots,q_n)\Omega}{\int dp_1\int dp_2\cdots\int dp_n\int dq_1\int dq_2\cdots\int dq_n\,\Omega} \tag{3}$$

and the partition function is

$$Z=\frac{1}{(2\pi\hbar)^{nd}}\int dp_1\int dp_2\cdots\int dp_n\int dq_1\int dq_2\cdots\int dq_n\,\Omega \tag{4}$$

in d dimensions. Fukuyama[14] proposed that the integration over momenta be regarded as defining an effective potential $\tilde{V}$:

$$Z=\frac{(2\pi mkT)^{nd/2}}{(2\pi\hbar)^{nd}}\int dq_1\int dq_2\cdots\int dq_n\, e^{-\beta\tilde{V}(q_1,q_2,\ldots,q_n)}\ , \tag{5}$$

i.e.,

$$e^{-\beta\tilde{V}}\equiv(2\pi mkT)^{-nd/2}\int dp_1\int dp_2\cdots\int dp_n\,\Omega\ . \tag{6}$$

To derive the effect of quantum fluctuations on the phonon spectrum, Fukuyama began with the electon lattice Hamiltonian (including cubic and quartic anharmonic terms in the potential) and worked out the dynamical matrix corresponding to the effective potential $\tilde{V}$ [computed via Eq. (6)]. The renormalized shear modulus is then derived from the long wavelength limit of the effective dynamical matrix. Thus, in Fukuyama's method, $\tilde{V}$ is treated as a *classical* potential which is supposed to generate *quantum* corrections to the dynamics.

We shall now offer a critique of this application of the effective potential. In general, from Eqs. (3)–(6) it follows that the ensemble average of a function of coordinates may be expressed as

$$\langle F(\hat{q}_1,\hat{q}_2,\ldots,\hat{q}_n)\rangle=\frac{\int dq_1\int dq_2\cdots\int dq_n\,F(q_1,q_2,\ldots,q_n)e^{-\beta\tilde{V}}}{\int dq_1\int dq_2\cdots\int dq_n e^{-\beta\tilde{V}}}\ , \tag{7}$$

but it is not obvious that $\tilde{V}$ describes the dynamical response of the system accurately. Since the Wigner distribution is but one of a host of possible phase-space distributions,[17,18] it is not clear why it should be selected for generating the effective potential. Employing some other phase-space distribution (e.g., the Kirkwood distribution[18,19]) would give a different $\tilde{V}$. In other words, $\tilde{V}$ is not unique. In fact, the effective potential is *not* an observable quantity. Only quantities which are obtained by integration over *both* momenta and coordinates [such as Z in Eq. (5)] qualify as observables, and in fact the same value for Z is obtained from a variety of effective potentials.[18] In other words, using Wigner's prescription for the definition of a distribution function, $\tilde{V}$ is to be regarded as a quantity which occurs at an *intermediate* stage of the calculation of such quantities as $\langle q\rangle$, and should not be assigned any physical significance *per se*. If one used, for example, Kirkwood's prescription for the definition of a distribution function, then a different quantity, $\tilde{V}_K$, say, would emerge which could be used to calculate the same value of such physical quantities as $\langle q\rangle$. The nonuniqueness in $\tilde{V}$ arises from the fact that when one uses a generalized distribution function,[20] $\Omega_g\equiv 0\Omega$, say, where 0 is an operator in phase space depending on derivatives with respect to momenta and coordinates, then a different effective potential emerges. However, the same physical results are again obtained,[20] since one also has to use the fact that $A_g=0^{-1}A$, where A and A_g are the classical phase-space quantities corresponding to an operator $\hat{A}$ in the Wigner and generalized distribution function approaches, respectively. By the same token, $\tilde{V}$ and $\tilde{V}_g$ are simply *parts* of H and H_g, where H and H_g are the classical phase-space quantities corresponding to the Hamiltonian $\hat{H}$, in the Wigner- and generalized-distribution function appraoches, respectively. It is to be emphasized[18] that $H_g\neq H$, which underlines the fact that the classical phase-space quantity corresponding to $\hat{H}$ should *not* be regarded as a classical Hamiltonian.

We will now illustrate our remarks by considering a one-dimensional anharmonic oscillator, subject to an external force γ, i.e., the Hamiltonian

$$H=\frac{p^2}{2m}+\tfrac{1}{2}m\omega_0^2q^2+\lambda q^4-\gamma q\ . \tag{8}$$

We shall be interested in the vibrational frequency of the oscillator as a function of temperature when $\gamma=0$; in applying the WDF it will, however, prove useful to examine the response to an applied force γ and set $\gamma=0$ at the end. Using the Wigner-Kirkwood expansion,[16,17] one readily finds

$$\Omega(q,p)=e^{-\beta H}\left\{1+\frac{\hbar^2\beta^2}{8m}\left[\left(\frac{\beta p^2}{3m}-1\right)(m\omega_0^2+12\lambda q^2)+\frac{\beta}{3}[(m^2\omega_0^4q^2+8\lambda m\omega_0^2q^4)-2\gamma(m\omega_0^2q+4\lambda q^3)]+O(\lambda^2,\gamma^2)\right]+O(\hbar^4)\right\}\ . \tag{9}$$

The meaning of the second and third terms in Eq. (9) is that they represent quantum corrections to the classical distribution $\exp(-\beta H)$. They arise from terms in the Wigner-Kirkwood expansion [see Eq. (2.82) of Ref. 17] involving derivatives of the potential appearing in Eq. (8).

When $\gamma=0$, Eq. (6) yields

$$\tilde{V}=\tfrac{1}{2}m\omega_0^2q^2+\lambda q^4-\frac{\hbar^2\beta}{8m}\left[-\tfrac{2}{3}m\omega_0^2+\left(\frac{\beta}{3}(m\omega_0^2)^2-8\lambda\right)q^2+\frac{8\beta}{3}m\omega_0^2\lambda q^4+O(\lambda^2)\right]+O(\hbar^4)\ . \tag{10}$$

Now according to Fukuyama's prescription, we must regard the coefficient of q^2 in $\tilde{V}$ as $\frac{1}{2}m\omega_R^2$, with ω_R the renormalized frequency. This is completely analogous to extracting the renormalized phonon frequencies from the effective dynamical matrix. Evidently, to first order in λ and $\hbar^2$,

$$\tfrac{1}{2}m\omega_R^2=\tfrac{1}{2}m\omega_0^2-\frac{\hbar^2\beta^2}{24}m\omega_0^4+\frac{\hbar^2\beta\lambda}{m}\ , \tag{11}$$

so that

$$\Delta=\omega_R-\omega_0=-\hbar^2\left(\frac{\beta^2\omega_0^2}{24}-\frac{\beta\lambda}{m^2\omega_0}\right)\ . \tag{12}$$

According to this result, quantum fluctuations cause a shift in the frequency of a *harmonic* oscillator ($\lambda=0$), which is of course absurd. Thus the effective potential gives an incorrect frequency even in the simplest case. In the electron

lattice calculation of Fukuyama there is also a frequency shift in the absence of anharmonicity [see Eq. (3.5) of Ref. 14], but this term does not contribute in the long wavelength limit.

The actual frequency shift of the oscillator whose Hamiltonian is given by Eq. (8) (with $\gamma=0$), is readily evaluated via the thermal Green's-function method. A computation paralleling the approach of Ref. 11 yields

$$\Delta=\frac{3\lambda\hbar}{m^2\omega_0^2}\coth\left(\frac{\beta\hbar\omega_0}{2}\right)+O(\lambda^2) \quad . \tag{13}$$

Expanding, one has

$$\Delta=\frac{6\lambda kT}{m^2\omega_0^3}+\frac{\lambda\beta\hbar^2}{2m^2\omega_0}+\cdots \quad . \tag{14}$$

The first term represents the shift due to thermal fluctuations, and the second is the lowest-order correction due to quantum fluctuations. The corresponding term in the effective potential result, Eq. (12), is too large by a factor of 2. In light of the failure of the effective potential method as applied to this elementary problem, there is no reason to believe the result for the electron lattice. *Ipso facto,* more elaborate calculations which consider the effect of a magnetic field[21] are also invalid.

The foregoing observations raise the following question: Can the frequency shift Δ be determined by means of the WDF? We believe that this may be accomplished in several ways, but for the present we consider only the following straightforward approach. If the frequency of an oscillator (in the limit of vanishing amplitude) is ω, then the response to an applied force γ is

$$\langle q\rangle_\gamma=\frac{\gamma}{m\omega^2}+O(\gamma^2) \quad . \tag{15}$$

Hence we take

$$\omega_R^2=\frac{\gamma}{m\langle q\rangle_\gamma} \quad (\gamma\to 0) \quad . \tag{16}$$

Using the WDF, Eq. (9), we find to first order in γ, λ, and $\hbar^2$

$$\langle q\rangle_\gamma=\frac{\gamma}{m\omega_0^2}\left(1-\frac{12\lambda}{m^2\omega_0^4\beta}-\frac{\lambda\beta\hbar^2}{m^2\omega_0^2}\right) \quad . \tag{17}$$

Equation (16) then yields

$$\Delta=\frac{6\lambda kT}{m^2\omega_0^3}+\frac{\lambda\beta\hbar^2}{2m^2\omega_0}+O(\lambda\hbar^4,\lambda^2) \tag{18}$$

in agreement with the Green's-function result. This result may also be obtained without the artifice of an external force, by using the WDF to compute the correlation function $\langle q(t)q(0)\rangle$. We have also used the WDF to obtain a result valid to all orders in $\hbar$ and first order in λ, which agrees with the more complete Green's-function result given in Eq. (13).

In conclusion, the discrepancy between the predictions of Refs. 13 and 14 regarding the effect of quantum fluctuations on the melting temperatures of the two-dimensional electron lattice has been shown to be an artifact of the "effective potential" method employed in Ref. 14. The effective potential is not valid for describing the dynamics of the system. In addition, our results have broader implications in that they establish the equivalence of using the Green's function or the WDF and, at least for the problem considered, we found that the use of the WDF method was conceptually and computationally simpler.

This research was partially supported by the Division of Materials Science, U.S. Department of Energy, under Grant No. DE-FG05-84ER45135.

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