Charge-density-wave instability in layered charged quantum liquids

A. Gold
Laboratoire de Physique des Solides, Université Paul Sabatier, 118 Route de Narbonne, 31062 Toulouse, France
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For boson and electron superlattices with a superlattice period d, analytical results for the local-field correction are derived within the Hubbard approximation. A charge-density-wave instability is found for a boson superlattice: $r_{sc} \propto d^{3/4}$. r_{sc} is the random-phase-approximation parameter r_s at the charge-density-wave instability. We discuss a recently proposed charge-density-wave instability in an electron superlattice and find $r_{sc} \propto d$.

Physical phenomena of the two-dimensional electron gas in layered structures are discussed in the literature.[1-4] Two-layer systems[1,2] and superlattices[3,4] can be realized in semiconductor heterostructures. A charge-density-wave (CDW) instability in electron superlattices for zero magnetic field[3] and large magnetic field[4] has been considered recently from a theoretical point of view. Boson systems represent a classic theoretical model system and are, however, much less studied.

In the following we show that a boson and a fermion superlattice at temperature zero is, at small density, unstable against the formation of a CDW. The ingredient of our theory is the random-phase approximation (RPA) with local-field correction (LFC).[5] By calculating the LFC for a superlattice we find that the static susceptibility of a superlattice is unstable below a certain density (or a certain superlattice period). We present analytical results for the LFC and the critical boson density. A similar phenomenon has been discussed for electron superlattices[3] and we report an analytical expression for the instability point in electron superlattices. We also discuss the implications of the approximation used in Ref. 3.

The particle-particle (electron or boson) Coulomb interaction in a superlattice is given by the interaction potential $V(q,q_z)$ in the Fourier space. q is the two-dimensional wave number. q_z is the wave number in z direction: $-\pi/d \leq q_z \leq \pi/d$. One finds[6]

$$V(q,q_z)=\frac{2\pi e^2}{q}\frac{\sinh(qd)}{\cosh(qd)-\cos(q_z d)} . \tag{1}$$

The same expression was derived for a boson superlattice.[7]

The RPA parameter r_s for the superlattice is described as $r_s^2=1/\pi N a^{*2}$.[5] $a^*=1/me^2$ is the Bohr radius. m is the boson mass (or the electron mass). We use for the Planck constant $h/2\pi=1$. We would like to mention that our calculation is for superlattices with ideal two-dimensional planes in the xy plane (no extension in z direction).

The RPA expression,[5] including the LFC $G(q,q_z)$, for the static susceptibility $\chi(q,q_z)$ of the superlattice is given by the susceptibility $\chi_0(q)$ of the free two-dimensional system (bosons or electrons) and the interaction potential as

$$\chi(q,q_z)=\frac{\chi_0(q)}{1+V(q,q_z)[1-G(q,q_z)]\chi_0(q)} . \tag{2}$$

The free-gas susceptibility is different for electrons and bosons. For a Bose condensate one finds[8,9]

$$\chi_0(q)=\frac{4mN}{q^2} . \tag{3}$$

The LFC takes into account short-range correlations in charged quantum liquids and classical liquids. The LFC leads to an improvement of the description over mean-field approximations like the RPA [with $G(q)=0$]. The LFC is most easily calculated within the Singwi-Tosi-Land-Sjölander (STLS) approach.[10] The Hubbard approximation for the LFC can easily be derived from this approach. This has been demonstrated for a three-dimensional electron gas[10] and a two-dimensional electron gas.[11] The LFC for a Bose condensate in two dimensions was discussed recently.[8,9] We have formulated the STLS approach for the self-consistent calculation of the LFC for superlattices. The derivation and the numerical results will be presented elsewhere.[12] From this calculation one can derive the LFC of a superlattice in Hubbard approximation in the same spirit as for the three- or two-dimensional electron gas. The relevant wave number in boson systems is different from the one in electron systems. For electron superlattices the relevant wave number is the Fermi wave number k_F. For the Bose gas it is the screening wave number q_s: $q_s=(8\pi N/a^*)^{1/3}$. a^* is the Bohr radius.

For a boson superlattice we find in the Hubbard approximation[12]

$$G_H(q,q_z)=r_s^{2/3}\frac{q}{[q^2+q_s^2]^{1/2}}\frac{\cosh(qd)-\cos(q_z d)}{\sinh(qd)} \times F_H(q,q_z) , \tag{4a}$$

with

$$F_H(q,q_z)=\frac{q^2+q_z^2-\sin(q_z d)(q_z/d)\mathrm{arccot}\{\sinh[(q^2+q_s^2)^{1/2}d]\}}{[q^2+q_z^2]} . \tag{4b}$$

We note that $F_H(q,q_zd=0)=F_H(q,q_zd=\pm\pi)=1$. For large d we get $q_z=0$ and we find $G_H(q,q_z)=qr_s^{2/3}/[q^2+q_s^2]^{1/2}$, the Hubbard LFC for the two-dimensional Bose condensate.[9] For large wave numbers we find $G_H(q\gg q_s,qd\gg 1,q_z)=r_s^{2/3}$. One can show that $G_H(q,q_zd=\pi/2)<r_s^{2/3}$: $G_H(q\ll q_s,qd\ll 1,q_zd=\pi/2)=2r_s^{2/3}\pi$ for $q_sd\ll 1$ and $G_H(q\ll q_s,qd\ll 1,q_zd=\pi/2)=r_s^{2/3}/q_sd$ for $q_sd\gg 1$. For small wave numbers we get

$$G_H(q\ll q_s,qd\ll 1,q_zd=\pi)=r_s^{2/3}\frac{2}{q_sd} . \quad (5)$$

From Eq. (5) we conclude that $G_H(q\ll q_s,qd\ll 1,q_zd=\pm\pi)$ increases with decreasing d.

The CDW instability occurs for $1/\chi(q_c,q_zd=\pi)=0$. For $1/\chi(q_c\sim 0,q_zd=\pi/2)$ no instability is observed. One can transfer this condition to the plasmon-dispersion relation $\omega_p(q,q_z)$: $\omega_p(q_c,q_zd=\pi)=0$ defines the instability point. The plasmon dispersion for boson superlattices with $G(q,q_z)=0$ was calculated in Ref. 7. With Eqs. (1)–(5) we derive for the instability point $1/\chi(q_c=0,q_zd=\pi)=0$,

$$r_{sc}=[d/a^*]^{3/4} . \quad (6)$$

For given superlattice period d one expects a Bose condensate for $r_s<r_{sc}$ and a CDW for $r_s>r_{sc}$. For given r_s the Bose condensate is stable for $d>d_c$ and a CDW with $q_c>0$ is expected for $d<d_c$.

For the free-electron gas in two dimensions the static susceptibility is written as

$$\chi_0(q)=\rho_F f(q) \quad (7)$$

with $f(q\le 2k_F)=1$ and $f(q>2k_F)=1-[1-4k_F^2/q^2]^{1/2}$.[13] $\rho_F=N/\varepsilon_F$ is the density of states at the Fermi energy ε_F. $N=k_F^2/2\pi$ is the electron density. The two-dimensional Thomas-Fermi screening wave number is given by $q_s=2\pi e^2\rho_F$ and does not depend on the electron density.

The LFC in the Hubbard approximation for an electron superlattice is expressed as[12]

$$G_H(q,q_z)=\frac{1}{2}\frac{q}{[q^2+k_F^2]^{1/2}}\frac{\cosh(qd)-\cos(q_zd)}{\sinh(qd)}\times F_H(q,q_z) , \quad (8a)$$

with

$$F_H(q,q_z)=\frac{q^2+q_z^2-\sin(q_zd)(q_z/d)\operatorname{arccot}[\sinh[(q^2+k_F^2)^{1/2}d]]}{[q^2+q_z^2]} . \quad (8b)$$

We observe that $F_H(q,q_zd=0)=F_H(q,q_zd=\pm\pi)=1$. For large d we recover the result for the two-dimensional electron gas:[11] $G_H(q)=q/[2(q^2+k_F^2)^{1/2}]$. For a large wave number we find $G_H(q\gg k_F,qd\gg 1,q_z)=\frac{1}{2}$. With Eq. (8) one can prove that $G_H(q,q_zd=\pi/2)<\frac{1}{2}$: $G_H(q\ll k_F,qd\ll 1,q_zd=\pi/2)=1/\pi$ for $k_Fd\ll 1$ and $G_H(q\ll k_F,qd\ll 1,q_zd=\pi/2)=1/(2k_Fd)$ for $k_Fd\gg 1$. For a small wave number we get for $q_zd=\pi$,

$$G_H(q\ll k_F,qd\ll 1,q_zd=\pi)=\frac{1}{k_Fd} . \quad (9)$$

The CDW instability occurs for $1/\chi(q_c,q_zd=\pi)=0$; no instability is found for $1/\chi(q,q_zd=\pi/2)$. This can be shown with Eq. (8). For an electron superlattice one gets $1/\chi(q_c=0,q_zd=\pi)=0$ for

$$r_{sc}=2^{1/2}[d/a^*+1] . \quad (10)$$

We notice that the d dependence of r_{sc} for an electron superlattice $r_{sc}\propto d$ is different from the one of a boson superlattice $r_{sc}\propto d^{3/4}$.

With Eq. (10) we find for $r_s=10$ and $r_s=20$ $d_c/a^*=6.1$ and $d_c/a^*=13.1$, respectively. The critical superlattice period found in Ref. 3 is very close to our result: $d_c/a^*=5.1$ for $r_s=10$ and $d_c/a^*=13.5$ for $r_s=20$. We conclude that Eq. (10) represents an analytical result for the CDW instability in electron superlattices.

However, one should keep in mind that the Hubbard approximation is not a very good approximation for $r_s>1$. The use of the Hubbard approximation implies that Eqs. (6) and (10) should only be applied for $r_s<1$: $d_c/a^*<1$. We believe, however, that the trend of our calculation is qualitatively correct even for $r_s>1$. More detailed results can be found in Ref. 12. Anyway, the discussed singularity occurs for every r_s if d is sufficiently small.

For a two-layer system with distance α we use for the susceptibility[3]

$$\chi_\pm(q)=\frac{\chi_0(q)}{1+\{V(q)[1-G(q)]\pm V_{12}(q)\}\chi_0(q)} , \quad (11)$$

with $V_{12}(q)=2\pi e^2\exp(-q\alpha)/q$ and $V(q)=2\pi e^2/q$. $G(q)$ is the LFC for the two-dimensional system. The instability point for the two-layer system is defined by $1/\chi_-(q_c)=0$. For $q_c=0$ we find for the boson-two-layer system

$$r_{sc}=[2\alpha/a^*]^{3/4} . \quad (12)$$

For the electron-two-layer system we get

$$r_{sc}=2^{1/2}[2\alpha/a^*+1] . \quad (13)$$

With Eq. (13) we find $\alpha_c/a^*=3.0$ (6.6) for $r_s=10$ (20). In Ref. 3 $\alpha_c/a^*=3.3$ (9.6) was found for $r_s=10$ (20). The 30% discrepancy for $r_s=20$ might be due to the use of the Hubbard approximation in our approach and finite-width effects neglected in our theory. α_c for two-layer systems is smaller than d_c for superlattices (for the same density) due to the stronger interaction potential in superlattices: every plane in a superlattice has two neighboring planes.

For the authors of Ref. 3 an expression of the LFC for a superlattice was not available. Therefore, they made the approximation $V(q,q_z)G(q,q_z)=V(q)G(q)$. Within this approximation they found $\chi(q,q_z)=\chi_0(q)/[1+V(q,q_z)\chi_0(q)-V(q)G(q)\chi_0(q)]$. We used the LFC for a superlattice. In order to get analytical results we applied the Hubbard approximation. Indeed, one can show that the two approaches for $\chi(q,q_z)$ give the same results for d_c, if in both approaches the Hubbard expression ($r_s<1$) for the LFC is used.[12] It is, however, unclear, whether this is still valid for $r_s>1$. Therefore, one might argue that the work in Ref. 3 for $r_s>1$ is not on a save basis.

The CDW instability found in the theoretical framework of Ref. 3 for electron superlattices must, from a mathematical point of view, be considered as an artificial instability: The authors did not realize that the LFC for a superlattice is singular for small d and this is the origin of the instability for $q_zd=\pi$. We claim, therefore, that we correctly calculated for the first time the CDW instability of a fermion superlattice.

For bosons we analyzed analytically the susceptibility and found that the instability at r_{sc} occurs for a finite q_c in a two-layer system and at $q_c=0$ for a superlattice. In our analytical derivation we assumed that the instability occurs at $q_c=0$. However, even for the two-layer system our analytical equations describe the instability point quite well: The numerically determined instability point r_{sc} was about 10% larger than the instability point derived from our analytical equation.

Can the discussed instability be important in the real world? Electron-two-layer systems[1,2] and electron superlattices[3,4] are realized with semiconductor heterostructures. Boson superlattices might be an important model system for high-T_c superconductors (for a review, see Ref. 14) and organic superconductors (for a review, see Ref. 15). The possible importance of Bose condensation in high-T_c superconductors was demonstrated recently in Ref. 16. In order to study the CDW instability we suggest to measure the plasmon dispersion $\omega_p(q,q_zd=\pi)$ in electron superlattices and in high-T_c superconductors. To the best of the author's knowledge such measurements have never been performed.

For a three-dimensional Bose condensate a transition to a Wigner crystal was predicted to occur for $r_{sW}\sim 160$.[17] Theoretical results for two dimensions are not available from the literature. We believe, however, that at small boson density a transition to a Wigner crystal can also be expected for boson superlattices. The interplay between the CDW and the Wigner crystal for electron superlattices was discussed in Ref. 3.

Before concluding we make some remarks on the effects of disorder on the proposed CDW instability. Disorder could pin the CDW (Ref. 18) and a transition from a superfluid Bose condensate to an insulating CDW would occur. Recently a disorder-induced superfluid-insulator transition was proposed for disordered boson superlattices.[7] The interplay between a (superfluid or localized) Bose condensate and a (pinned or unpinned) CDW is certainly very interesting. Similar remarks hold for the electron superlattice. The interplay between the CDW instability and the metal-insulator transition could be very important in semiconductor superlattices.

In conclusion we have shown that a charge-density-wave instability exists in a layered Bose condensate and in layered electron systems for $q_zd=\pi$. Analytical results for the density of this instability have been presented. Essential for the instability is the existence of many-body corrections (local-field correction) to the random-phase approximation for charged quantum liquids. We presented analytical results for the local-field correction in the Hubbard approximation. This Brief Report points out that qualitatively new phenomena are expected in *microscopically layered charged quantum liquids* due to a many-body effect.

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[1]G. S. Boebinger, H. W. Jiang, L. N. Pfeiffer, and K. W. West, Phys. Rev. Lett. **64**, 1793 (1990).
[2]A. H. MacDonald, P. M. Platzman, and G. S. Boebinger, Phys. Rev. Lett. **65**, 775 (1990).
[3]L. Swierkowski, D. Neilson, and J. Szymanski, Phys. Rev. Lett. **67**, 240 (1991).
[4]X. M. Chen and J. J. Quinn, Phys. Rev. Lett. **67**, 895 (1991).
[5]D. Pines and P. Nozières, *The Theory of Quantum Liquids* (Benjamin, New York, 1966), Vol. I.
[6]A. L. Fetter, Ann. Phys. (N.Y.) **88**, 1 (1974).
[7]A. Gold, Z. Phys. B **81**, 155 (1990).
[8]C. I. Um, W. H. Kahng, E. S. Yim, and T. F. George, Phys. Rev. B **41**, 259 (1990).
[9]A. Gold, Z. Phys. B **83**, 429 (1991).
[10]K. S. Singwi, M. P. Tosi, R. H. Land, and A. Sjölander, Phys. Rev. **176**, 589 (1968).
[11]M. Jonson, J. Phys. C **9**, 3055 (1976).
[12]A. Gold, Z. Phys. B **86**, 193 (1992).
[13]F. Stern, Phys. Rev. Lett. **18**, 546 (1967).
[14]R. Micnas, J. Ranninger, and S. Robaszkiewicz, Rev. Mod. Phys. **62**, 113 (1990).
[15]D. Jérome, Science **252**, 1509 (1991).
[16]A. Gold and A. Mlayah, Physica C **181**, 374 (1991).
[17]D. Ceperley and B. J. Alder, Phys. Rev. Lett. **45**, 566 (1980).
[18]G. Grüner, Rev. Mod. Phys. **60**, 1129 (1988).