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Sum rules for the planar surface of stabilized jellium

Adam Kiejna
Institute of Experimental Physics, University of Wrocław, Plac M.Borna 9, 50-204 Wrocław, Poland

Paul Ziesche*
Institut Romand de Recherche Numerique en Physique des Materiaux, Lausanne, Switzerland

Roland Kaschner
Technische Universität Dresden, Institut für Theoretische Physik, D-01069 Dresden, Mommsenstrasse 13, Germany

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The Hellmann-Feynman sum rules for the planar surface of *s*-*p*-bonded metals modeled by a half-space-stabilized jellium are presented and numerically tested. They relate density derivatives of the (stabilized) bulk and surface energies to moments of the electric field appearing in the metal region, to the number of electrons spilled out into the vacuum region, and to the electronic density at the surface.

I. INTRODUCTION

The progress in the calculation of the electronic surface properties of metals observed over the last three decades has been accompanied by the derivation of several exact relations and sum rules[1-5] involving bulk and surface quantities. These exact relations were derived by the application of the uniform background (jellium) model of (*s*-*p*-bonded) metal surfaces. (For the modification of the sum rules for crystalline systems cf. also the addition in Ref. 5.) The jellium model describes well basic features of the inhomogeneous electron gas near the metal surface and allows us to treat the problem numerically without, relatively, great computational expense. The exact relations or theorems prove to be useful checks on the consistency of such numerical calculations. It is important that jellium calculations require one input parameter only, namely, the average electron density in the bulk. Also, the calculated surface properties depend on this parameter solely. This nice property of jellium is overshadowed by the fact that jellium is in mechanical equilibrium only for the average electron density $\overline{n}$ corresponding to $r_s \approx 4.2$, where $\overline{n} = 3/4\pi r_s^3 a_0^3$. In addition to this, the instability of jellium is manifested by the negative surface energies for high density metals ($r_s \lesssim 2.5$).[6]

Recently, Perdew, Tran, and Smith,[7] and independently Shore and Rose,[8] have proposed the stabilized-jellium model which retains the simplicity of jellium (i.e., depends on r_s only) and stabilizes it for all r_s by introducing a structureless pseudopotential correction.[9] Applied to the metal-surface problem the stabilized jellium gives very encouraging results:[7,8,10-12] the calculated surface energy is positive in the whole range of metallic r_s and fits well to the experimental data.

In the present paper we derive the stabilized-jellium counterparts of the exact "bulk-surface" and "surface-surface" relations for jellium.[4,5] In Sec. II we summarize the essential formulas for stabilized jellium. Section III presents the many-electron Hamiltonian of the stabilized jellium and the derivation of the theorems. In Sec. IV the results of numerical checks of the theorems are presented. The last section gives a summary.

II. THE STABILIZED JELLIUM MODEL

For the sake of further discussion it is convenient to summarize the essential expressions for the stabilized jellium model. Here we will follow the structureless pseudopotential formulation of the problem by Perdew, Tran, and Smith.[7] The total energy of a (finite) system as a functional of the electron density $n(\mathbf{r})$ and the positive background density $n_+(\mathbf{r}) = \overline{n}\,\Theta_{\mathcal{V}}(\mathbf{r})$, binding $N = \overline{n}\mathcal{V}$ electrons, is given by

$$E[n(\mathbf{r}), n_+(\mathbf{r})] = E_{\text{jell}}[n(\mathbf{r}), n_+(\mathbf{r})] + (\varepsilon_M + \overline{w}_R)\int d^3r\, n_+(\mathbf{r}) + \langle \delta v\rangle_{\text{WS}} \int d^3r\, \Theta_{\mathcal{V}}(\mathbf{r})[n(\mathbf{r}) - n_+(\mathbf{r})]. \tag{1}$$

The Heaviside step function $\Theta_{\mathcal{V}}(\mathbf{r})$ equals 1 for $\mathbf{r}$ inside $\mathcal{V}$ and 0 for $\mathbf{r}$ outside $\mathcal{V}$. E_{jell} is the total energy of the (ordinary, i.e., nonstabilized) jellium and includes standard kinetic, electrostatic, and exchange-correlation terms. The two terms added to E_{jell} describe the stabilization. They contain (i) the average Madelung energy of point ions (of valency Z) embedded in a uniform negative background,

$$\varepsilon_M(\overline{n}) = -\frac{9}{10}\frac{Z^{2/3}}{r_s}\frac{\epsilon^2}{a_0}, \tag{2}$$

with $\epsilon^2 = e^2/4\pi\varepsilon_0$ and $a_0 = \hbar^2/m\epsilon^2$; (ii) the (averaged) Ashcroft pseudopotential contribution

$$\overline{w}_R(\bar{n}, r_c) = 2\pi\epsilon^2\bar{n}r_c^2; \tag{3}$$

(iii) a "difference potential"

$$\langle\delta v\rangle_{\text{WS}} = \bar{n}\frac{\partial}{\partial\bar{n}}[\varepsilon_M(\bar{n}) + \overline{w}_R(\bar{n}, r_c)], \tag{4}$$

being the average over the Wigner-Seitz sphere of the difference between the pseudopotential of the lattice of ions and the electrostatic potential of the uniform positive background. For the details of the averaging procedure see Ref. 7.

Now the Ashcroft pseudopotential radius r_c is chosen by demanding the bulk energy, which corresponds to the functional (1),

$$\varepsilon(\bar{n}, r_c) = \varepsilon_0^{\bar{n}} + \varepsilon_M(\bar{n}) + \overline{w}_R(\bar{n}, r_c), \tag{5}$$

to have its minimum for the (experimentally or theoretically) given equilibrium density n_0 of the particular (s-p-bonded) metal under consideration. The first term is the usual jellium bulk energy

$$\varepsilon_0^{\bar{n}} \equiv t_0(\bar{n}) + \varepsilon_{\text{XC}}(\bar{n}), \tag{6}$$

where $t_0(\bar{n})$ and $\varepsilon_{\text{XC}}(\bar{n})$ represent the kinetic and exchange-correlation contributions, respectively. The minimum condition

$$\left.\frac{\partial}{\partial\bar{n}}\varepsilon(\bar{n}, r_c)\right|_{\bar{n}=n_0} = 0 \tag{7}$$

leads [using $\varepsilon_M(\bar{n}) \sim \bar{n}^{1/3}$] to an expression for the Ashcroft radius r_c as a function of n_0:

$$2\pi\epsilon^2[r_c(n_0)]^2 = -\left[\frac{1}{3}\frac{\varepsilon_M(n_0)}{n_0} + \frac{d\varepsilon_0^{n_0}}{dn_0}\right]. \tag{8}$$

In this way the total energy (1) depends on the material parameters n_0 and Z and on the actual background density $\bar{n}$, which may agree with n_0 (for the case of equilibrium, i.e., zero pressure) or not (nonzero pressure).

With $r_c(n_0)$ from Eq. (8) the bulk energy (5) of the stabilized jellium is now denoted as

$$\begin{aligned} \varepsilon_{n_0}^{\bar{n}} &= \varepsilon_0^{\bar{n}} + \Delta\varepsilon_{n_0}^{\bar{n}}, \\ \Delta\varepsilon_{n_0}^{\bar{n}} &= \varepsilon_M(\bar{n}) + \overline{w}_R(\bar{n}, r_c(n_0)), \end{aligned} \tag{9}$$

where the subscripts n_0 and 0 refer to stabilized and nonstabilized jellium, respectively. Thus the minimum condition (7) can be written as

$$\left.\frac{\partial\varepsilon_{n_0}^{\bar{n}}}{\partial\bar{n}}\right|_{\bar{n}=n_0} = 0 \quad \text{or} \quad \frac{d\varepsilon_0^{n_0}}{dn_0} = -\left.\frac{\partial\Delta\varepsilon_{n_0}^{\bar{n}}}{\partial\bar{n}}\right|_{\bar{n}=n_0} \tag{10}$$

and the functional (1) takes the form

$$\begin{aligned} E[n, n_+] = {} & E_{\text{jell}}[n, n_+] + \Delta\varepsilon_{n_0}^{\bar{n}}N \\ & + \bar{n}\frac{\partial\Delta\varepsilon_{n_0}^{\bar{n}}}{\partial\bar{n}}\int d^3r\,\Theta_{\mathcal{V}}(\mathbf{r})[n(\mathbf{r}) - \bar{n}]. \end{aligned} \tag{11}$$

From this functional results an effective one-particle potential for the Kohn-Sham equation,

$$v_{n_0}^{\bar{n}}(\mathbf{r}) = \frac{\delta}{\delta n(\mathbf{r})}\{E[n(\mathbf{r}), n_+(\mathbf{r})] - T_s[n(\mathbf{r})]\},$$

where $T_s[n(\mathbf{r})]$ is the noninteracting kinetic energy. The potential $v_{n_0}^{\bar{n}}(\mathbf{r})$ differs from $v_0^{\bar{n}}(\mathbf{r})$, the corresponding quantity for the nonstabilized jellium, according to

$$v_{n_0}^{\bar{n}}(\mathbf{r}) = v_0^{\bar{n}}(\mathbf{r}) + \Delta\varepsilon_{n_0}^{\bar{n}} + \bar{n}\frac{\partial\Delta\varepsilon_{n_0}^{\bar{n}}}{\partial\bar{n}}[\Theta_{\mathcal{V}}(\mathbf{r}) - 1]. \tag{12}$$

The third term on the right-hand side (rhs) describes a discontinuity of the potential $v_{n_0}^{\bar{n}}(\mathbf{r})$. Just this jump in the effective potential stabilizes the jellium; cf. also the discussion of Shore and Rose.[8] In the special case $\bar{n} = n_0$ the jump amounts to $n_0\,d\varepsilon_0^{n_0}/dn_0$ because of Eq. (10).

With the ("stabilized") potential (12) the solutions of the Kohn-Sham equations for each considered stabilized jellium yield the electronic density and the total energy in the same way as for the nonstabilized potential $v_0^{\bar{n}}(\mathbf{r})$, but the results are of course different due to the changed effective one-particle potential.

III. THE HAMILTONIAN AND THE THEOREMS

For the nonstabilized half-space jellium from the Hellmann-Feynman theorem sum rules for the derivatives of the bulk and the surface energy with respect to the background density ("bulk-surface" and "surface-surface" theorems) have been (re)derived,[4,5,13] generalizing corresponding Budd-Vannimenus theorems. To repeat this procedure for the stabilized jellium, we need the many-body Hamiltonian, which corresponds to the energy functional (11). From the expressions presented above it is obvious that the Hamiltonian is given by

$$\begin{aligned} H_{n_0}^{\bar{n},\mathcal{V}} = {} & H_0^{\bar{n},\mathcal{V}} + \Delta\varepsilon_{n_0}^{\bar{n}}N \\ & + \bar{n}\frac{\partial\Delta\varepsilon_{n_0}^{\bar{n}}}{\partial\bar{n}}\int d^3r\,\Theta_{\mathcal{V}}(\mathbf{r})[\hat{n}(\mathbf{r}) - \bar{n}] \end{aligned} \tag{13}$$

with $\hat{n}(\mathbf{r}) = \sum_i \delta(\mathbf{r} - \mathbf{r}_i)$ being the electron density operator.

With this Hamiltonian, we proceed similarly as in the derivation of the sum rules for jellium (see Refs. 4 and 5), i.e., we do the following.

(i) Start with a finite geometry (a cylinder or disk with radius A and thickness $2L$).

(ii) Consider first the limit of an extended slab ($A \to \infty$) and then the limit of a half-space jellium ($L \to \infty$).

(iii) Specify the Hellmann-Feynman theorem to appropriate scalings of the positive background ($\bar{n}$) and to the material parameter n_0.

The application of the Hellmann-Feynman theorem and the above procedure lead to the final formulas where derivatives of the bulk energy $\varepsilon_{n_0}^{\bar{n}}$ and of the surface energy $\sigma_{n_0}^{\bar{n}}$ with respect to $\bar{n}$ and n_0 are related to moments of the electric field and the electron density profile.

The resulting sum rules can be summarized as follows:

(i) The scaling of $\bar{n}$ in the bulk energy yields

$$n_{n_0}^{\bar{n}}(0)\frac{\partial\Delta\varepsilon_{n_0}^{\bar{n}}}{\partial\bar{n}} = \int_{-\infty}^{0} dz\,E_{n_0}^{\bar{n}}(z) - \bar{n}\frac{d\varepsilon_0^{\bar{n}}}{d\bar{n}}, \tag{14}$$

where $n_{n_0}^{\overline{n}}(z)$ and $E_{n_0}^{\overline{n}}(z)$ are, respectively, the electronic density and the electric field of a semi-infinite stabilized jellium with the background extending from $z \to -\infty$ to $z = 0$. $n_{n_0}^{\overline{n}}(0)$ is, therefore, the electronic density at the surface ($z = 0$).

This sum rule (14) can be considered as an analog to the Budd-Vannimenus ("bulk-surface") theorem[1,5]

$$n_0 \frac{d\varepsilon_0^{n_0}}{dn_0} = \int_{-\infty}^{0} dz\, E_0^{n_0}(z) \tag{15}$$

for the nonstabilized jellium. For a stabilized jellium at its equilibrium density $\overline{n} = n_0$ Eq. (14) can be rewritten in the form

$$[n_0 - n_{n_0}^{n_0}(0)] \frac{d\varepsilon_0^{n_0}}{dn_0} = \int_{-\infty}^{0} dz\, E_{n_0}^{n_0}(z), \tag{16}$$

where Eq. (10) is used. It is easy to see that Eq. (16) coincides with the "generalized Budd-Vannimenus theorem" (F14) of Monnier and Perdew[14] if their quantity C (variational parameter) is chosen as the stabilizing prefactor $\langle \delta v \rangle_{\mathrm{WS}}$ at $\overline{n} = n_0$, i.e., as $-n_0\, d\varepsilon_0^{n_0}/dn_0$, and their X is set to zero. A comparison of the sum rules (14) and (16) with the original Budd-Vannimenus theorem (15) shows that they differ by an extra term proportional to the electronic density at the surface, $n_{n_0}^{n_0}(0)$, and by replacing $E_0^{n_0}(z) \to E_{n_0}^{n_0}(z)$.

(ii) The scaling of $\overline{n}$ in the surface energy $\sigma_{n_0}^{\overline{n}}$ yields

$$\frac{\partial}{\partial \overline{n}} \sigma_{n_0}^{\overline{n}} = \int_{-\infty}^{0} dz\, z E_{n_0}^{\overline{n}}(z) - \left(\frac{\partial}{\partial \overline{n}} \overline{n} \frac{\partial}{\partial \overline{n}} \Delta \varepsilon_{n_0}^{\overline{n}} \right) \int_{0}^{\infty} dz\, n_{n_0}^{\overline{n}}(z). \tag{17}$$

This sum rule corresponds to the Vannimenus-Budd ("surface-surface") theorem for the nonstabilized jellium[2,5]

$$\frac{d}{dn_0} \sigma_0^{n_0} = \int_{-\infty}^{0} dz\, z E_0^{n_0}(z). \tag{18}$$

The difference terms in the theorems (14) and (17), compared with the expressions for the nonstabilized case, result from the stabilization terms appearing in the Hamiltonian (13).

(iii) Application of a change of n_0 in the Hellmann-Feynman theorem yields

$$\frac{\partial}{\partial n_0} \sigma_{n_0}^{\overline{n}} = \overline{n} \left(\frac{\partial^2 \varepsilon_{n_0}^{\overline{n}}}{\partial \overline{n}^2} \right)_{n_0} \int_{0}^{\infty} dz\, n_{n_0}^{\overline{n}}(z). \tag{19}$$

For the derivation of this formula we used amongst other things the relation

$$-\left(\frac{\partial^2 \varepsilon_{n_0}^{\overline{n}}}{\partial \overline{n}^2} \right)_{n_0} = \frac{\partial^2 \Delta \varepsilon_{n_0}^{\overline{n}}}{\partial n_0\, \partial \overline{n}}, \tag{20}$$

which follows trivially from Eq. (7) using Eq. (3), i.e., with $\overline{w}_R(\overline{n}, r_c(n_0)) = \overline{n}\, f(n_0)$.

For $\overline{n} = n_0$ the sum of the theorems (14) and (17) yields after some simple manipulations

$$\frac{d}{dn_0} \sigma_{n_0}^{n_0} = \int_{-\infty}^{0} dz\, z E_{n_0}^{n_0}(z) + \left(\frac{d}{dn_0} n_0 \frac{d}{dn_0} \varepsilon_0^{n_0} \right) \int_{0}^{\infty} dz\, n_{n_0}^{n_0}(z). \tag{21}$$

The last term of Eqs. (17), (19), and (21) contains the number of electrons (per unit area) spilled out into the vacuum region.

Finally, we want to mention that in analogy to the "surface-edge" theorems, which we have derived for the nonstabilized jellium recently,[5,15] such sum rules can be obtained for the stabilized case too. So as for the ordinary (nonstabilized) jellium also for the stabilized jellium there exists a hierarchy of sum rules leading from bulk via surfaces to edges (and even corners[13]).

IV. NUMERICAL CHECKS OF THE THEOREMS

The validity of the stabilized jellium sum rules derived above has been tested numerically using the Monnier-Perdew version[13] of the Lang-Kohn computer code. Assuming that the uniform positive background occupies the left half-space, i.e., $n_+(\mathbf{r}) = \overline{n}\Theta(-z)$, the Kohn-Sham problem was solved self-consistently with the effective potential including the stabilizing term $\overline{n}(\partial \Delta \varepsilon_{n_0}^{\overline{n}} / \partial \overline{n}) \Theta(-z)$ on the metal side. The surface energy functional consists of jellium (kinetic, electrostatic, and exchange-correlation) terms plus the stabilized jellium contribution resulting from the last term on the right-hand side of Eq. (1). The jellium terms are influenced by stabilization only indirectly. The exchange and correlation energy was calculated in the local-density approximation and for the correlation energy the parametrized[16] values of Ceperley and Alder[17] have been used.

The calculations were performed for four representative metals with the r_s values covering the whole range of metallic densities. For the numerical integration over the wave number k an integration mesh with $\Delta(k/k_F) = 0.01$ is taken. The real space region of computation extended from $-3.5\lambda_F$ to $2.0\lambda_F$ with the integration mesh spaced by $\Delta(x/\lambda_F) = 0.005$ where $\lambda_F = 2\pi/k_F$ is the Fermi wavelength. To assure a good convergency of the quantities, in each calculation 100 iterations were used.

The results are presented in Table I for several values of the actual density parameter r_s (corresponding to $\overline{n}$) for each metal, which is characterized by the equilibrium density parameter r_{s0} (with $n_0 = 3/4\pi r_{s0}^3 a_0^3$). In columns 3 and 4 we give the numerical values of the two sides of Eq. (14). The integral over the electric field $E_{n_0}^{\overline{n}}$ inside the metal, appearing in Eq. (14), has been determined through the electrostatic potential difference between the surface and the bulk according to the relation

$$\int_{-\infty}^{0} dz\; E^{\overline{n}}_{n_0}(z) = \phi(0) - \phi(-\infty). \tag{22}$$

Here $\phi(0)$ and $\phi(-\infty)$ denote, respectively, the values of electrostatic potential at the uniform background edge and in the bulk. The comparison of the numerical values of the left- and right-hand sides of Eq. (14) shows excellent agreement both for polyvalent (Al, Mg) and monovalent (Na, Cs) metals. The deviations are lower than 0.3%.

Columns 5 and 6 of Table I contain the numerical results for Eq. (17) connecting the derivative of the surface energy, with respect to the uniform electron density $\overline{n}$, with the integral over the electric field. The surface energy derivative, appearing in this relation, was evaluated numerically. The integral standing on the right-hand side of Eq. (17) was determined from the following relation for the integral of the electrostatic potential $\phi(z)$:

$$-\int_{-\infty}^{0} dz\; zE^{\overline{n}}_{n_0}(z) = \int_{-\infty}^{0} dz\;[\phi(z) - \phi(-\infty)]. \tag{23}$$

As in the previous case both sides of Eq. (17) agree very well. The agreement is best for the high density metals. Generally, the deviations are very small and in the worst case do not exceed 3.2%. It is interesting to note that the derivative of the surface energy with respect to $\overline{n}$ changes its sign and becomes positive with the decrease of the actual density. This means that the surface energy attains a minimum for a certain value of r_s. The r_s minimizing the surface energy does not coincide with the r_{s0} characterizing the bulk equilibrium and generally exceeds r_{s0}.

For a given r_{s0} the number of electrons spilling out into the vacuum, determined by the integral appearing in the last term on the rhs of Eq. (17), is decreasing with the increase of r_s. This decrease is smaller, however, than the corresponding increase in the value of the integrated electrostatic potential [Eq. (23)] which eventually prevails and causes the derivative of the surface energy to increase with r_s.

The results of the numerical tests of Eq. (19) are given in columns 7 and 8 of Table I. Similarly, as for Eq. (17) the derivative of the surface energy with respect to n_0 was calculated numerically. The displayed numbers show perfect fulfillment of this sum rule. For the densities considered the left- and right-hand sides of Eq. (19) do not differ by more than 0.5%. The derivative of the surface energy with respect to the equilibrium density n_0 is a decreasing function of r_s and does not change its sign. Both the prefactor appearing on the rhs of Eq. (19) and the integrated electron density on the vacuum side are positive and decreasing functions of r_s.

V. SUMMARY

The results of several recent papers[7,8,10–12] seem to support the opinion that the stabilized-jellium model provides a more realistic description of the properties of *s-p* bonded metals than ordinary jellium does. In this paper we demonstrated how the sum rules for the (nonstabilized) jellium are modified if one applies the stabilization procedure.

Considering the density derivatives of the bulk and surface energies, for the stabilized jellium we have to distinguish between the equilibrium density (n_0) of the particular metal under consideration and the actual density ($\overline{n}$), which may be different from the former one (nonzero pressure) or not (zero pressure). Our results are as follows.

(i) For the derivative of the bulk energy we have obtained Eq. (14), which is a modification of the "bulk-surface" (or Budd-Vannimenus) theorem, relating bulk

TABLE I. The numerical values for the left-hand sides (lhs's) and right-hand sides (rhs's) of the sum rules (14), (17), and (19) of a half-space stabilized jellium. All quantities are given in atomic units (energies in hartrees).

Metal		Eq. (14)		Eq. (17)		Eq. (19)	
r_{s0}	r_s	lhs	rhs	lhs	rhs	lhs	rhs
Al	1.80	-0.012338	-0.012341	-0.154321	-0.154171	0.184007	0.184162
2.07	2.07	-0.039325	-0.039326	-0.058592	-0.058554	0.072278	0.072296
	2.40	-0.050362	-0.050366	0.003206	0.003180	0.027212	0.027193
Mg	2.30	0.002348	0.002350	-0.102914	-0.102930	0.138370	0.138555
2.65	2.65	-0.017163	-0.017164	-0.031704	-0.031688	0.053954	0.053938
	3.00	-0.024941	-0.024945	0.007597	0.007597	0.023887	0.023830
Na	3.70	0.004323	0.004324	-0.026211	-0.026201	0.056515	0.056475
3.99	3.99	-0.000899	-0.000900	-0.005376	-0.005379	0.034261	0.034225
	4.30	-0.004417	-0.004420	0.010434	0.010502	0.020941	0.020846
Cs	5.40	0.005909	0.005907	-0.011919	-0.011776	0.042374	0.042194
5.63	5.63	0.003436	0.003436	-0.001345	-0.001304	0.031523	0.031447
	5.90	0.001209	0.001207	0.008543	0.008624	0.022681	0.022578

and surface properties, but with an extra term proportional to the electronic density at the surface. (The obtained theorem for the derivative of the bulk energy with respect to n_0 instead of $\overline{n}$ is a trivial relation.)

(ii) The surface energy derivative with respect to the actual density $\overline{n}$ is given by Eq. (17), which is the counterpart of the "surface-surface" (or Vannimenus-Budd) theorem for jellium and contains an extra term proportional to the number of electrons (per unit area) that spill out into the vacuum region. The derivative of the surface energy with respect to the equilibrium density n_0 is given by Eq. (19), i.e., it is also proportional to the number of electrons outside the electronic surface. The two theorems (17) and (19) for the derivative of the surface energy involve the second derivative of the bulk energy.

By solving self-consistently the Kohn-Sham equations for a semi-infinite stabilized jellium, these new sum rules (14), (17), and (19) have been tested numerically. The results of Sec. IV show that they are very well satisfied. Hence, these sum rules can be applied for checking the self-consistency of numerical calculations and to get further insight into the physics of the stabilization procedure at planar surfaces.

The sum rule (14) is used in a recent attempt[18] to study spherical voids within stabilized jellium (as a model for spherical-like vacancy clusters in *s*-*p*-bonded metals). Besides this, the stabilized analogs to the nonstabilized jellium-void theorems[4,19,20] can be derived. Similarly, one can derive sum rules for edges and corners of the stabilized jellium.

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[*] Permanent address: Many-Body Problems Group, P.O. Box 410113, D-01224 Dresden, Germany.

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