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Virial equations for extended electron systems in a homogeneous magnetic field: a jellium model and a periodic solid

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Abstract. A model N -electron system—a finite jellium—is considered first. The virial equation (VE) for it is obtained by adapting the result of Holas and March (Holas A and March N H 1999 *Phys. Rev. A* **60** 2853) concerning a molecule in a homogeneous magnetic field B . Next, by applying a limiting procedure with N tending to infinity, the VE for an infinite-jellium system is established. This result extends the well-known zero-field VE by adding a term involving a derivative over B . Similarly, the VE for a periodic solid is obtained by applying a limiting procedure to the VE for a cluster ('finite crystal'). All VEs are valid for the systems in arbitrary (ground or excited) eigenstates.

1. Introduction

The area of atoms, molecules, and condensed phases in intense magnetic fields is of considerable current interest. For atoms and molecules, astrophysical interest is high, because chemistry can be altered, for instance, in the very high magnetic fields found at the surface of neutron stars (Lieb *et al* 1992, Freeman and March 1996). In condensed phases, n-type InSb in an intense magnetic field was studied theoretically in early work (Durkan *et al* 1968). This motivated experiments by Andrei *et al* (1988) in the area relating to the theory of a two-dimensional electron liquid in a transverse magnetic field (Laughlin 1983, Isihara 1989); see also March (1996).

This motivation, plus the very recent theoretical investigation of Steinberg and Ortner (1998, 1999) on the correlation energy of an electron gas (in the so-called jellium model) at high density in an intense magnetic field has led us back to the virial theorem for such a system, and to seek the generalization of the (zero-magnetic-field) result of March (1958); see also Argyres (1967):

$$-r_s \frac{d\epsilon_{\text{jel}}(r_s)}{dr_s} = 2\epsilon_{\text{kin}}(r_s) + \epsilon_{\text{pot}}(r_s) \quad (1.1)$$

where ϵ_{kin} , ϵ_{pot} , and ϵ_{jel} are, respectively, the kinetic, potential, and total ground-state (GS) energy per electron of the jellium model,

$$\epsilon_{\text{jel}} = \epsilon_{\text{kin}} + \epsilon_{\text{pot}} \quad (1.2)$$

and r_s is the usual parameter related to the electron density n as

$$n(r_s) = \left(\frac{4}{3}\pi r_s^3\right)^{-1}. \quad (1.3)$$

Atomic units are used throughout, with the bohr a_0 , the hartree $\hbar^2/(ma_0^2)$, and $\hbar/(ea_0^2) = 2.3505 \times 10^5$ T as the units of length, energy, and magnetic field, respectively.

For the jellium placed in a homogeneous magnetic field \mathbf{B} we expect equation (1.1) to be extended by a term involving the derivative over B , similar to one involving r_s :

$$-r_s \frac{\partial \epsilon_{\text{jel}}(r_s, B)}{\partial r_s} + \alpha B \frac{\partial \epsilon_{\text{jel}}(r_s, B)}{\partial B} = 2\epsilon_{\text{kin}}(r_s, B) + \epsilon_{\text{pot}}(r_s, B). \quad (1.4)$$

In order to check this conjecture on some example and to determine the value of the parameter α , let us consider a uniform high-density electron gas in an extremely high-field regime, where the potential energy can be neglected compared with the kinetic energy ϵ_{MTF} , which is connected, for the motion in the plane $\perp \mathbf{B}$, with occupying the orbitals of the lowest Landau level, and with free motion along \mathbf{B} . Thus, in this regime,

$$\epsilon_{\text{pot}}(r_s, B) \rightarrow 0 \quad (1.5a)$$

$$\epsilon_{\text{kin}}(r_s, B) \rightarrow \epsilon_{\text{MTF}}(r_s, B) = c'_{\text{MTF}} r_s^{-6} B^{-2}. \quad (1.5b)$$

We shall term $\epsilon_{\text{MTF}}(r_s, B)$ the magnetic Thomas–Fermi (MTF) kinetic energy, to underline its origin as having the same phase-space basis (Kadomtsev 1970), but now in the high-field limit, as the original zero-field statistical model. Its form can be found, e.g., in Lieb *et al* (1992) and Steinberg and Ortner (1998, 1999).

After simple algebra we find that equation (1.4) is satisfied by equation (1.5) together with (1.2) when $\alpha = 2$. In section 3 it will be proven that the conjectured virial equation (1.4) with $\alpha = 2$ is true for arbitrary r_s and arbitrary B .

2. Results for the finite-jellium system

We define the finite jellium as a system of N mutually interacting electrons, moving in a homogeneous magnetic field \mathbf{B} , and interacting with the ‘background’: the positive charge of the value N smeared uniformly over a finite volume Ω . This system resembles a molecule in which discrete nuclei are replaced by a continuous background. Therefore we propose to use the Holas and March (1999) (HM) results on the virial equation (VE) for a molecule in a magnetic field. But we must first determine how their final result must be modified by the above-mentioned replacement.

In the notation of HM, their equations (3.9), (3.10),

$$E_{\text{mol}} = T + E_C \quad (2.1a)$$

represents the total eigenenergy of a molecule (here—the finite jellium) in the GS or some excited state, with T the kinetic energy term, and

$$E_C = E_{\text{ee}} + E_{\text{en}} + E_{\text{nn}} \quad (2.1b)$$

the potential energy, a sum of all contributions due to Coulombic (C) interactions: electron–electron, electron–nucleus, and nucleus–nucleus. In terms of the density distribution $n_+(\mathbf{r})$ of the background charge, the last term in the case of jellium can be written as

$$E_{\text{nn}} = \frac{1}{2} \int d^3 r_1 d^3 r_2 \frac{n_+(\mathbf{r}_1)n_+(\mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|} \quad (2.2)$$

(the analogue of the molecular E_{nn} , equation (3.8) of HM), while the potential needed for E_{en} (equation (3.6) of HM) is

$$v_{\text{en}}(\mathbf{r}) = - \int d^3 r' \frac{n_+(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \quad (2.3)$$

(the analogue of equation (3.1) of HM). Let the shape of the region occupied by the background charge be characterized by a function $\kappa(\vartheta, \varphi) > 0$ such that, in the spherical coordinates,

$$n_+(r, \vartheta, \varphi) = \frac{N}{\Omega(R)} \Theta(R\kappa(\vartheta, \varphi) - r) \quad (2.4)$$

where $\Theta(x)$ is the unit step function, while R is a parameter describing the linear dimension of the region (e.g., by choosing $\kappa(\vartheta, \varphi) = 1$, a sphere of the radius R is defined). As follows directly from equation (2.4), the volume of the background region (BR) is

$$\Omega(R) = \int d^3r \Theta(R\kappa(\vartheta, \varphi) - r) = R^3 \Omega(1). \quad (2.5)$$

It will be convenient to characterize the finite jellium by r_s connected with the uniform density of the BR

$$\frac{N}{\Omega(R)} = n(r_s) \quad (2.6)$$

and by N . So, by combining equations (1.3), (2.6), and (2.5), we find

$$R(r_s, N) = (N^{\frac{4}{3}} \pi r_s^3 / \Omega(1))^{1/3} = r_s N^{1/3} R(1, 1). \quad (2.7)$$

Therefore, with $n_+(r, \vartheta, \varphi; r_s, N)$ given by equation (2.4) together with (2.6) and (2.7), the dependence on $\{r_s, N\}$ in equations (2.2) and (2.3) is revealed to be

$$E_{\text{nn}}(r_s, N) = r_s^{-1} N^{5/3} E_{\text{nn}}(1, 1) \quad (2.8)$$

$$v_{\text{en}}(\mathbf{r}; r_s, N) = r_s^{-1} N^{2/3} v_{\text{en}}(\mathbf{r}/(r_s R(1, N)); 1, 1). \quad (2.9)$$

We are now ready to investigate scaling properties of these quantities: the identity obtained from equation (2.9)

$$v_{\text{en}}(\lambda \mathbf{r}; r_s, N) = \lambda^{-1} (\lambda r_s^{-1}) N^{2/3} v_{\text{en}}(\mathbf{r}/((\lambda^{-1} r_s) R(1, N)); 1, 1) = \lambda^{-1} v_{\text{en}}(\mathbf{r}; \lambda^{-1} r_s, N) \quad (2.10)$$

leads to

$$\left. \frac{\partial}{\partial \lambda} v_{\text{en}}(\lambda \mathbf{r}; r_s, N) \right|_{\lambda=1} = - \left(1 + r_s \frac{\partial}{\partial r_s} \right) v_{\text{en}}(\mathbf{r}; r_s, N) \quad (2.11)$$

while the direct differentiation of equation (2.8) gives

$$-r_s \frac{\partial}{\partial r_s} E_{\text{nn}}(r_s, N) = E_{\text{nn}}(r_s, N). \quad (2.12)$$

Equations (2.11) and (2.12) are analogues of equations (3.4) and (3.11) of HM: we see that the former ones can be obtained from the last ones by applying the replacement

$$\mathbf{R} \cdot \frac{\partial}{\partial \mathbf{R}} \longrightarrow r_s \frac{\partial}{\partial r_s}. \quad (2.13)$$

With this replacement, the VE (4.8b) of HM reads (see also equation (2.1a) here)

$$\left(-r_s \frac{\partial}{\partial r_s} + 2B \frac{\partial}{\partial B} \right) E_{\text{mol}}(r_s, N, B) = 2T(r_s, N, B) + E_{\text{C}}(r_s, N, B). \quad (2.14)$$

This is an exact result for the VE of the finite jellium. It should be noted that the VE obtained by HM was shown to be valid for an arbitrary (ground or excited) eigenstate of a molecule. Therefore, the same is true also in the case of the finite-jellium result (2.14). To simplify notation, we have suppressed the dependence of all energy terms on the label (a set of quantum numbers) of the eigenstate, on the shape function κ of the BR, and on the orientation \mathbf{B}/B of the magnetic field with respect to this region.

On putting $B = 0$, equation (2.14) reduces to the GS result of Argyres (1967) (his 'free boundary conditions' case), and generalizes his result to an arbitrary eigenstate.

3. Results for the infinite-jellium system

Let us consider now a sequence (numbered by N) of the finite-jellium systems, which all have the same density (the same r_s) of the BR together with its shape function κ and its orientation with respect to \mathbf{B}/B , and all are in the eigenstate with the same label. It should be noted that the volume Ω occupied by the uniform background of each N -electron system is proportional to N : $\Omega(r_s, N) \propto R^3(r_s, N) \propto Nr_s^3$, while the volume $\partial\Omega$ of the ‘skin’ (a layer of thickness of a few r_s above and below the surface of the BR) shows weaker dependence on N : $\partial\Omega(r_s, N) \propto r_s R^2(r_s, N) \propto N^{2/3}r_s^3$. Consider the local (at the space point \mathbf{r}) characteristics of the electron system—the one-particle density matrix $\gamma_1(\mathbf{r} + \mathbf{r}', \sigma_1; \mathbf{r} + \mathbf{r}'', \sigma_2)$ and the pair density $n_2(\mathbf{r} + \mathbf{u}/2, \mathbf{r} - \mathbf{u}/2)$ —the information sufficient to evaluate the total energy; see HM. Because in the space far outside the surface these characteristics are exponentially small, while within the skin they may differ essentially from the bulk characteristics, the relative contribution of these two regions to the total energy diminishes with increasing N . Therefore we conclude that the limit of the total eigenenergy per electron

$$\epsilon_{\text{jel}}(r_s, B) = \lim_{N \rightarrow \infty} \frac{E_{\text{mol}}(r_s, N, B)}{N} \quad (3.1)$$

and, similarly, the limit $\epsilon_{\text{kin}}(r_s, B)$ obtained from $T(r_s, N, B)$ and the limit $\epsilon_{\text{pot}}(r_s, B)$ from $E_C(r_s, N, B)$ —all exist and are independent of the particular shape function κ and field direction. Moreover, we conclude that there exist the limits of both sides of equation (2.14) divided beforehand by N :

$$\left(-r_s \frac{\partial}{\partial r_s} + 2B \frac{\partial}{\partial B} \right) \epsilon_{\text{jel}}(r_s, B) = 2\epsilon_{\text{kin}}(r_s, B) + \epsilon_{\text{pot}}(r_s, B). \quad (3.2)$$

This VE is our main result concerning the (infinite-) jellium model (called also the zero-temperature electron plasma). When combined with equation (1.2) (which is the large- N limit of equation (2.1a) divided by N ; see also equation (3.1)), equation (3.2) allows for separation of the kinetic and potential energy contributions in terms of the total energy (compare equation (2) of March (1958) and equations (2), (3) of Argyres (1967), both in the zero-field case):

$$\epsilon_{\text{kin}}(r_s, B) = \left(-r_s \frac{\partial}{\partial r_s} + 2B \frac{\partial}{\partial B} - 1 \right) \epsilon_{\text{jel}}(r_s, B) \quad (3.3a)$$

$$\epsilon_{\text{pot}}(r_s, B) = \left(+r_s \frac{\partial}{\partial r_s} - 2B \frac{\partial}{\partial B} + 2 \right) \epsilon_{\text{jel}}(r_s, B). \quad (3.3b)$$

From the fact that the VE (3.2) is valid for an arbitrary eigenstate of the jellium system it follows, in particular, that this VE can be applied to each of the possible phases (in the $\{r_s, B\}$ plane) of the GS of the jellium. As found by MacDonald and Bryant (1987) (see also references therein), the transition on the phase diagram from the uniform-density state to the Wigner-crystal state occurs in several steps.

4. High-density jellium in a strong magnetic field

The results obtained in the previous section for a jellium of arbitrary density n in an arbitrary magnetic field B in some eigenstate will be applied now to the GS of this system at high density and in a strong magnetic field—the case investigated recently by Steinberg and Ortner (1998, 1999) (SO). General features of the electronic motion in this regime were already summarized in section 1 (below equation (1.4)). It is convenient to describe this uniform system like SO in terms of two variables: the expansion parameter $r_B \propto k_F^{-1} \propto (l_B^2 n)^{-1}$, and the filling parameter $t = \epsilon_F / (\hbar \omega_c)$, where $l_B = (\hbar / (eB))^{1/2}$ is the magnetic length, $\omega_c = eB/m$ is the cyclotron

frequency, and k_F, ϵ_F are the Fermi momentum and energy, connected with one-dimensional free motion. The direct and reciprocal variable transformations

$$r_B(r_s, B) = \pi^{-2} 3^{-1} 2 r_s^3 B \quad t(r_s, B) = \pi^2 3^2 2^{-3} r_s^{-6} B^{-3} \quad (4.1a)$$

$$r_s(r_B, t) = (3\pi^4)^{1/3} r_B t^{1/3} \quad B(r_B, t) = (2\pi^2)^{-1} r_B^{-2} t^{-1} \quad (4.1b)$$

induce the function transformations $\epsilon \longleftrightarrow \tilde{\epsilon}$, so

$$\tilde{\epsilon}(r_B, t) = \epsilon(r_s(r_B, t), B(r_B, t)) \quad (4.2a)$$

$$\epsilon(r_s, B) = \tilde{\epsilon}(r_B(r_s, B), t(r_s, B)). \quad (4.2b)$$

Let us find now the transformed VE (3.2). By applying the chain rule of differentiation we obtain

$$\begin{aligned} \frac{\partial \epsilon(r_s, B)}{\partial \ln(r_s)} &= \left(\frac{\partial \ln(r_B)}{\partial \ln(r_s)} \frac{\partial}{\partial \ln(r_B)} + \frac{\partial \ln(t)}{\partial \ln(r_s)} \frac{\partial}{\partial \ln(t)} \right) \tilde{\epsilon}(r_B, t) \\ &= \left(+3 \frac{\partial}{\partial \ln(r_B)} - 6 \frac{\partial}{\partial \ln(t)} \right) \tilde{\epsilon}(r_B, t) \end{aligned} \quad (4.3a)$$

$$\frac{\partial \epsilon(r_s, B)}{\partial \ln(B)} = \left(+1 \frac{\partial}{\partial \ln(r_B)} - 3 \frac{\partial}{\partial \ln(t)} \right) \tilde{\epsilon}(r_B, t). \quad (4.3b)$$

We see that the combination of the above results

$$\left(-\frac{\partial}{\partial \ln(r_s)} + 2 \frac{\partial}{\partial \ln(B)} \right) \epsilon(r_s, B) = \left(-\frac{\partial}{\partial \ln(r_B)} + 0 \frac{\partial}{\partial \ln(t)} \right) \tilde{\epsilon}(r_B, t) \quad (4.4)$$

allows for rewriting the VE (3.2) in a simpler form:

$$-r_B \frac{\partial}{\partial r_B} \tilde{\epsilon}_{\text{jel}}(r_B, t) = 2\tilde{\epsilon}_{\text{kin}}(r_B, t) + \tilde{\epsilon}_{\text{pot}}(r_B, t). \quad (4.5)$$

Consequently, equation (3.3) transforms into

$$\tilde{\epsilon}_{\text{kin}}(r_B, t) = \left(-r_B \frac{\partial}{\partial r_B} - 1 \right) \tilde{\epsilon}_{\text{jel}}(r_B, t) \quad (4.6a)$$

$$\tilde{\epsilon}_{\text{pot}}(r_B, t) = \left(+r_B \frac{\partial}{\partial r_B} + 2 \right) \tilde{\epsilon}_{\text{jel}}(r_B, t). \quad (4.6b)$$

The results (4.5) and (4.6) are valid for arbitrary (but nonzero) r_s, B . Moreover, they remain true also for more general transformations: $r_B = c_1 r_s^{1+2\alpha} B^\alpha$, $t = c_2 r_s^{2\beta} B^\beta$, where α, β, c_1, c_2 are arbitrary real constants satisfying $\beta \neq 0, c_1 \neq 0, c_2 \neq 0$.

The results of SO for the expanded ϵ_{jel} are valid for a small enough expansion parameter, say $r_B \lesssim \eta \ll 1$ (where η is a chosen small number), and for a limited filling, $t \leq 1$. These inequalities, rewritten in terms of r_s, B , are: $r_s \lesssim 6.636\eta$, and $2.231r_s^{-2} \leq B \lesssim 14.80\eta r_s^{-3}$. Within this validity range, SO obtained the GS energy of the jellium in a field as a series in r_B (analogous to the well-known zero-field series in r_s), a sum of terms called the MTF kinetic, exchange, and correlation energy:

$$\tilde{\epsilon}_{\text{jel}}(r_B, t) = \tilde{\epsilon}_{\text{MTF}}(r_B, t) + \tilde{\epsilon}_x(r_B, t) + \tilde{\epsilon}_c(r_B, t) \quad (4.7a)$$

$$\tilde{\epsilon}_{\text{MTF}}(r_B, t) = c_{\text{MTF}} r_B^{-2} \quad c_{\text{MTF}} = (6\pi^2)^{-1} \quad (4.7b)$$

$$\tilde{\epsilon}_x(r_B, t) = c_x(t) r_B^{-1} \quad (4.7c)$$

$$\tilde{\epsilon}_c(r_B, t) = c_{\text{cl}}(t) \ln(r_B) + c_{\text{c0}}(t) + c_{\text{ch}}(r_B, t). \quad (4.7d)$$

A form of the (higher-order) term $c_{\text{ch}}(r_B, t)$ is unknown, but it vanishes when $r_B \rightarrow 0$. All t -dependent coefficients can be found in SO. With the help of equation (4.6), we obtain from

the SO series (4.7) the correlated kinetic and potential energies as

$$\tilde{\epsilon}_{\text{kin}}(r_B, t) = \tilde{\epsilon}_{\text{MTF}}(r_B, t) - \left(r_B \frac{\partial}{\partial r_B} + 1 \right) \tilde{\epsilon}_c(r_B, t) \quad (4.8a)$$

$$\tilde{\epsilon}_{\text{pot}}(r_B, t) = \tilde{\epsilon}_x(r_B, t) + \left(r_B \frac{\partial}{\partial r_B} + 2 \right) \tilde{\epsilon}_c(r_B, t). \quad (4.8b)$$

5. Results for a periodic solid

Periodicity of a crystal (solid) will be described by elementary translations $\{\mathbf{a}_j = r_{\text{UC}} \mathbf{a}_j^0: j = 1, 2, 3\}$, where the dimensionless vectors \mathbf{a}_j^0 satisfy, by definition, $(\mathbf{a}_1^0 \times \mathbf{a}_2^0) \cdot \mathbf{a}_3^0 = 1$. The crystal unit cell (UC), of the volume $\Omega_{\text{UC}} = r_{\text{UC}}^3$, is a parallelepiped spanned on \mathbf{a}_j . It contains M_{UC} nuclei of charges Z_μ at positions $\boldsymbol{\rho}_\mu = \sum_j \rho_{\mu j} \mathbf{a}_j$, $\mu = 1, \dots, M_{\text{UC}}$. To maintain neutrality, there must be $N_{\text{UC}} = \sum_\mu Z_\mu$ electrons per UC.

We define now a cluster ('finite crystal') as a system of $N = N_1 N_2 N_3 N_{\text{UC}}$ interacting electrons moving in a homogeneous magnetic field \mathbf{B} and interacting with the nuclear framework contained in $N_1 N_2 N_3$ UCs. The array of nuclear positions is

$$\mathbf{R} = \{ \{ \{ \mathbf{R}_{l_1 l_2 l_3 \mu}: \mu = 1, \dots, M_{\text{UC}} \}: l_j = 1, \dots, N_j \}: j = 1, 2, 3 \}$$

where $\mathbf{R}_{l_1 l_2 l_3 \mu} = r_{\text{UC}} \sum_j (l_j + \rho_{\mu j}) \mathbf{a}_j^0$, while the array of nuclear charges is

$$\mathbf{Z} = \{ \{ Z_\mu: \mu = 1, \dots, M_{\text{UC}} \}: l = 1, \dots, (N_1 N_2 N_3) \}.$$

All nuclear positions are fixed and, possibly, unrelaxed. The nucleus–nucleus interaction energy is included. We see that this cluster is identical with a molecule considered by HM, with the parameter r_{UC} playing the role of their size parameter R . Therefore the VE (4.13b) of HM holds. In the present notation it reads

$$\left(-r_{\text{UC}} \frac{\partial}{\partial r_{\text{UC}}} + 2B \frac{\partial}{\partial B} \right) E_{\text{mol}}^{\mathbf{N}}(r_{\text{UC}}, B) = 2T^{\mathbf{N}}(r_{\text{UC}}, B) + E_{\text{C}}^{\mathbf{N}}(r_{\text{UC}}, B) \quad (5.1)$$

where $E_{\text{mol}}^{\mathbf{N}}$ represents the total energy of a molecule (here—the cluster characterized by $\mathbf{N} = (N_1, N_2, N_3)$) in some eigenstate; see equation (2.1) for its decomposition.

Consider next a sequence (labelled with \mathbf{N}) of clusters which all have the same r_{UC} , \mathbf{a}_j^0 , M_{UC} , $\rho_{\mu j}$, Z_μ , \mathbf{B} , and their state label. By arguments given in section 3 we conclude that the limit of the total eigenenergy per UC

$$\epsilon_{\text{UC}}(r_{\text{UC}}, B) = \lim_{\{N_j \rightarrow \infty: j=1,2,3\}} \frac{E_{\text{mol}}^{\mathbf{N}}(r_{\text{UC}}, B)}{N_1 N_2 N_3} \quad (5.2)$$

exists, and, similarly, limits of its components and the VE (5.1)—all divided by $N_1 N_2 N_3$ —exist:

$$\left(-r_{\text{UC}} \frac{\partial}{\partial r_{\text{UC}}} + 2B \frac{\partial}{\partial B} \right) \epsilon_{\text{UC}}(r_{\text{UC}}, B) = 2\epsilon_{\text{kin}}(r_{\text{UC}}, B) + \epsilon_{\text{pot}}(r_{\text{UC}}, B). \quad (5.3)$$

This VE is our main result for a periodic solid in an arbitrary (ground or excited) state. The relations analogous to equation (3.3) hold too. By recalling that the pressure p in a system of the energy ϵ_{UC} and the volume Ω_{UC} is given by $p = -\partial \epsilon_{\text{UC}} / \partial \Omega_{\text{UC}}$, and remembering that $\Omega_{\text{UC}} = r_{\text{UC}}^3$, we can replace the term $-r_{\text{UC}} \partial \epsilon_{\text{UC}}(r_{\text{UC}}, B) / \partial r_{\text{UC}}$ by $3\Omega_{\text{UC}}(r_{\text{UC}}) p(r_{\text{UC}}, B)$.

A summary is given in the abstract.

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